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Revision of the DELFIC Particle Activity Module

September 2010

Prepared by
David A. Hooper
Vincent J. Jodoin

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Nuclear Science and Technology Division

REVISION OF THE DELFIC PARTICLE ACTIVITY MODULE

David A. Hooper
Vincent J. Jodoin

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ABBREVIATIONS

ABEGN	fission yield data file used in 1968 and 1979 versions of DELFIC
ASA	Atmospheric Science Associates
BATMAN	subroutine in DELFIC that solves the Bateman equations for decay
BREAKUP.DAT	data file created by SAIC to store the nuclide information
DELFIC	DEfense Land Fallout Interpretive Code
DNA	Defense Nuclear Agency
ENDF/B-VII	Evaluated Nuclear Data Files B, version 7
ERM	exposure rate multipliers: used by DELFIC to convert activity density to exposure rate
FORTRAN	IBM Mathematical FORmula TRANslation System: program language of DELFIC
IT	Isomeric Transition (formerly gamma decay)
MULT	list of powers of 8 in DELFIC (8, 64, 512 … 8^{11})
Masstab	array in BREAKUP.DAT for storing mass numbers
Nattab	array in BREAKUP.DAT for storing atomic numbers
NUCLID	original DELFIC array to store coded nuclide information
Nuclida	array in BREAKUP.DAT for storing coded atomic numbers and mass numbers
Nuclidb	array in BREAKUP.DAT for storing coded decay information
Nuclidc	array in BREAKUP.DAT for storing coded branching information
ORIGEN	Oak Ridge Isotope Generation
PAMDAT1	subroutine created in 1992 for storing nuclear data other than those in NUCLID
SAIC	Science Applications International Corporation: revised DELFIC in 1992
TAPE20.DAT	electronic version of ABEGN: contains 1979 version of fission yields
YIELD	subroutine in 1968 DELFIC that adjusted fission yields for branch merging

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David Hooper

SUMMARY

In 1968, the Defense Land Fallout Interpretive Code (DELFIC) was created to model fallout patterns and provide assistance in nuclear explosion modeling efforts in an effort sponsored by the Defense Atomic Support Agency. Originally written in FORTRAN IV, DELFIC provided a remarkably efficient method to estimate land activity and exposure patterns for user-specified weather and nuclear device parameters. The program has been maintained relatively intact since its inception, with only two revisions of note for the purposes of this paper. In 1979, DELFIC was revised by Atmospheric Science Associates for the Defense Nuclear Agency (DNA); this revision streamlined certain computational sections (particularly the processing of decay chains) and simplified the user manual. Then in 1992, Science Applications International Corporation revised DELFIC at the request of DNA. The 1992 revisions expanded the exposure rate multiplier database and made revisions to the processing of decay chains. (Other revisions have been made to DELFIC throughout its life, but no other revisions are relevant to this report and are omitted from discussion.)

With the heightened concerns regarding nuclear proliferation and nuclear incidents in the first decade of the twenty-first century, interest has been generated in enhancing DELFIC's ability to model nuclear explosions and their fallout patterns to provide greater defense planning and disaster recovery support. With this goal in mind, several extensive modifications have been planned for DELFIC. This report catalogues efforts to improve the decay engine and nuclear database within DELFIC.

The first section of this report will discuss the historical development of DELFIC. In this section, the problematic history of a phenomenon termed "branch merging" will be investigated, the coding scheme for storing nuclear data will be explained, and the fission yields will be discussed. An argument for the revision of each aforementioned topic will also be presented and a solution will be proposed.

The second section of this report will discuss upgrades made to DELFIC in 2008 by Oak Ridge National Laboratory. Particular attention will be paid to three goals of that upgrade: replacement of the nuclear database with information from ENDF/B-VII; expansion of the robustness of the decay engine through modification of the nuclide coding system; and establishment of a final resolution to the problems with branch merging. Verification results will be included to demonstrate the effectiveness of the revisions. Known limitations will be discussed to facilitate future revisions, if such revisions are desired.

ABSTRACT

The Defense Land Fallout Interpretive Code (DELFIC) was originally released in 1968 as a tool for modeling fallout patterns and for predicting exposure rates. Despite the continual advancement of knowledge of fission yields, decay behavior of fission products, and biological dosimetry, the decay data and logic of DELFIC have remained mostly unchanged since inception. Additionally, previous code revisions caused a loss of conservation of radioactive nuclides. In this report, a new revision of the decay database and the Particle Activity Module is introduced and explained. The database upgrades discussed are replacement of the fission yields with ENDF/B-VII data as formatted in the Oak Ridge Isotope Generation (ORIGEN) code, revised decay constants, revised exposure rate multipliers, revised decay modes and branching ratios, and revised boiling point data. Included decay logic upgrades represent a correction of a flaw in the treatment of the fission yields, extension of the logic to include more complex decay modes, conservation of nuclides (including stable nuclides) at all times, and conversion of key variables to double precision for nuclide conservation. Finally, recommended future work is discussed with an emphasis on completion of the overall radiation physics upgrade, particularly for dosimetry, induced activity, decay of the actinides, and fractionation.

1. BACKGROUND AND DEVELOPMENT

1.1 INTRODUCTION

In the Defense Land Fallout Interpretive Code (DELFIC), decay of fission products is analytically calculated by the Bateman equations for radioactive decay. To facilitate this process, DELFIC first allocates all fission products into monolithic decay based on the fission yields and on the decay patterns of the nuclides. Then the Bateman equations are used for exact solutions to the monolithic chains, and the results are reassembled for output processing.

Investigation into the DELFIC decay engine focused on three aspects: (1) treatment of monolithic decays that have decays to common daughters (branch merging), (2) the coding system used to store nuclide information and generate the monolithic chains, and (3) the fission yield data themselves. Regarding the first aspect, studying the history and development of DELFIC's decay engine revealed that the issue of branch merging has been problematic and requires clarification in the code and in the documentation. It is hoped that this report will provide a final solution to this problem and will clarify the issue for future users of DELFIC. Regarding the second aspect, studying the nuclide coding system revealed two significant findings: limitations of the decay engine prevented DELFIC (in its unrevised form) from accepting updated fission yield and decay information, and the actual capabilities of the coding system allow for more flexibility than was previously supposed. This report will explain both findings in order to develop solutions that allow the DELFIC nuclide library to be revised with contemporary fission yield and decay data from the ENDF/B-VII data. Finally, with regard to the third aspect, studying the fission yield data showed that the existing fission yield files did not reliably or accurately conserve the number of fission products very accurately.

This study was performed with the hopes of demonstrating that DELFIC can readily be improved to accept more thorough and up-to-date information for fission yield and radioactive decay. The findings of this study then served as justification for these updates in the DELFIC logic, as they are outlined in the second half of this report.

1.2 BACKGROUND

In a fission reaction, the nucleus of the fissioning atom divides into two (occasionally three) smaller nuclei referred to as fission products. Because the ratio of neutrons to protons (the N/Z ratio) in large stable atoms tends to be greater than that in lighter stable atoms, the fission products tend to have high N/Z ratios relative to their size. These high N/Z ratios make most fission products unstable, leading to much of the radioactivity present after a fission event occurs.

Several modes of decay may be exhibited by the various fission fragments and their daughters. Owing to the high N/Z ratio, beta decay is the most common decay mode. In beta decay, a neutron is transformed into a proton, an electron, and an antineutrino. The electron and antineutrino escape the nucleus, typically at high rates of speed. Another common decay mode is isomeric transition (IT), in which the nucleus releases excess energy in the form of a gamma ray. A somewhat less common decay is beta-neutron (b-n) decay, in which the nucleus releases a neutron in addition to the process of beta decay. Unlike beta decay and IT, b-n decay reduces the mass number of the nucleus by one. Electron capture decay is even less common than b-n decay. When electron capture occurs, an inner shell orbital electron is absorbed into the nucleus, causing a proton to transform into a neutron and causing a neutrino to be released. Alpha decay is another very rare mode of decay for fission products. In alpha decay, the nucleus releases a particle consisting of two protons and two neutrons—an alpha particle. Other, more "exotic" modes of decay exist for fission products but are extremely rare. In both the original DELFIC decay library and the ORIGEN

(Oak Ridge Isotope Generation) library discussed in this report, these decays are not represented. For each mode of decay, the daughter nucleus of the decay may be explicitly predicted from the parent. For example, for all nuclei that decay by beta decay, the daughter will have one less neutron and one more proton than the parent.

The time at which an individual nuclide decays is a random event, but the decay behavior of large numbers of atoms of an isotope may be modeled statistically. From the statistical model, the half-life of a radioactive nuclide may be determined to describe the rate at which those atoms decay. Since this is valid for all radioactive nuclides, the decays of any nuclide and its subsequent daughters may be modeled in decay chains. The decay chains, modeled mathematically by the Bateman equations, provide a description of the decay behavior of radioactive atoms over time and are used to model the decay of fission products after fission occurs.

Many fission products and fission product daughters may have more than one possible mode of decay. In these cases, the decay modes are typically modeled with single decay constant and branching ratios. The branching ratios describe the percentage of decays of a given isotope that undergo a specific mode of decay. For example, ^{138}I has a decay constant of 4.623E–4 s^{-1}; it may decay either by beta decay or by electron capture. Since 93.1% of all ^{138}I atoms eventually undergo beta decay, the branching ratio for beta decay is 0.931, and the branching ratio for electron capture is 0.069. With the decay constant and the branching ratios, both the decay rate and the rates of production of all decay daughters may be determined. Since many fission fragments and their subsequent daughters have multiple modes of decay, the decay chains of the products of fission events are very complex and interwoven. Not only do many parents decay into multiple daughters, but many daughters may each be produced by the decay of multiple parents.

DELFIC models the decay of fission products explicitly through the Bateman equations. If the yield and magnitude of a fission event are known, the number of atoms of each fission product isotope is entered into the Bateman equations for the decay chains of the fission products. The decay of the fission products is then modeled exactly over time, thus allowing the activity of the fission products to be calculated at any point in time after the fission event. However, the modeling process is complicated by the multiple modes of decay that many isotopes undergo. In fact, managing the decay chains has proved to be one of the more problematic aspects of the revision history for the DELFIC code. In this report, the history of decay chain modeling will be investigated and a solution to the revision histories will be illustrated.

1.3 BRANCH MERGING

1.3.1 A Brief Statement of the Problem

"Branch merging," as it shall be termed throughout this paper, is the condition in which a daughter nuclide can be obtained through multiple decay paths. For example, Fig. 1 illustrates a simple case in which nuclide A decays to nuclide C via beta decays while nuclide B decays to nuclide C via b-n decay. For the purpose of visualization, initial yield values are arbitrarily assigned so that the yield of A is 10, the yield of B is 20, and the yield of C is 50 (atoms per 10,000 fissions).

DELFIC simplifies the decay process by first creating monolithic decay chains to represent every possible path of decay from the fission products. As a result, some nuclides appear in multiple chains. In Fig. 1, nuclide C would appear in two chains, one with nuclide A and one with nuclide B. Since nuclide C appears in multiple chains, its initial yield cannot be allocated to every decay chain that C inhabits. Otherwise, in this example, DELFIC would assign the fission yield (50 atoms/10,000 fissions in Fig. 1) for nuclide C twice, resulting in an erroneously high initial inventory of nuclide C.

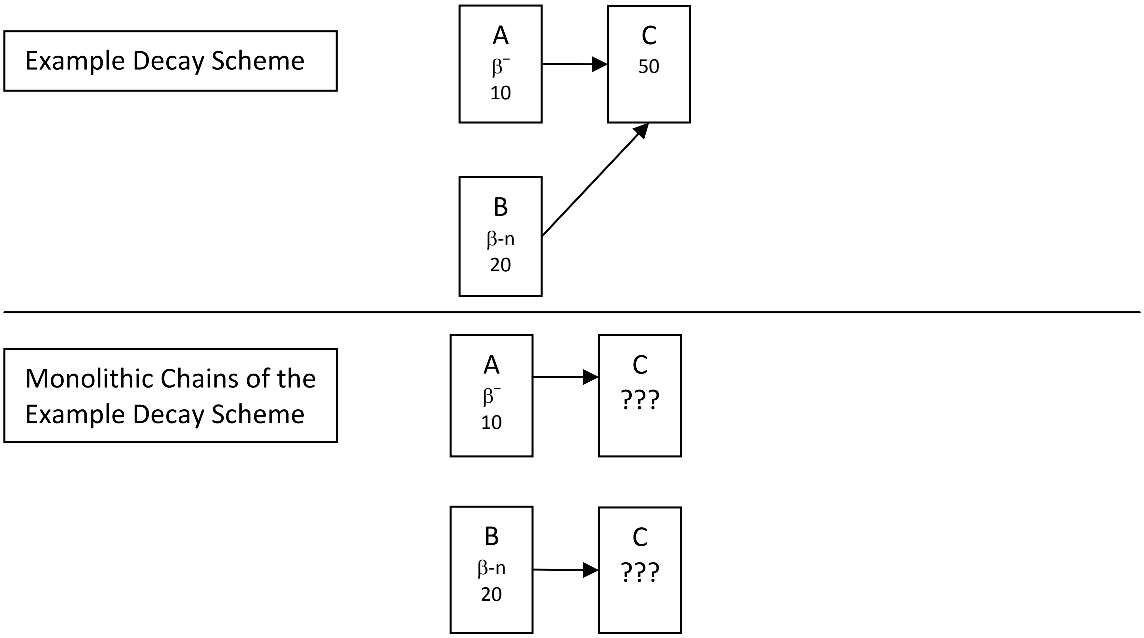


Fig. 1. Branch merging example.

1.3.2 Original Treatment of Branch Merging

In the 1968 version of DELFIC, branch merging was accounted for through the use of the subroutine YIELD. This subroutine was called before BATMAN was used and adjusted the yields of all nuclides affected by branch merging to conserve overall yields. In this manner, the fission yields stored in the data tapes for 1968 DELFIC were the true fission yields as they were known at the time. In the yield units of DELFIC—atoms per 10,000 fissions—these yields would theoretically add to 20,000 for a fission type.

1.3.3 1979 Treatment of Branch Merging—ABEGN Modification

In the 1979 version of DELFIC, the subroutine YIELD was removed. Since the decay paths were the same for all runs, the YIELD subroutine produced identical corrections to the fission yields for every execution of the program. To save computational time and memory, the adjustments previously performed by YIELD were applied to the yields in the data file ABEGN. In this manner, DELFIC no longer needed to perform a correction for branch merging because the data file was adjusted *a priori*. Since the yields are reduced by integer factors equal to the number of paths to a nuclide, the yields in this modified system would add to a number less than 20,000 atoms per 10,000 fissions.

Two case studies are provided in Fig. 2 and Fig. 3 to illustrate the differences between the 1968 and 1979 yield data. First, the beta-decay chain for mass number 133 is shown with actual fission yield data from DELFIC 1968 (Fig. 2). In the 1979 data, the fission yields have been divided by the number of paths from the start of a chain to a particular nuclide (Fig. 3).

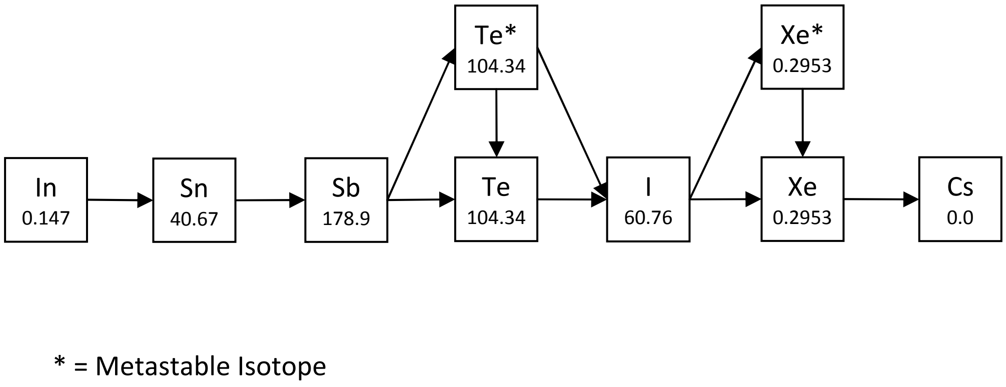


Fig. 2. 1968 fission yields for mass chain 133 (Tompkins 1968).

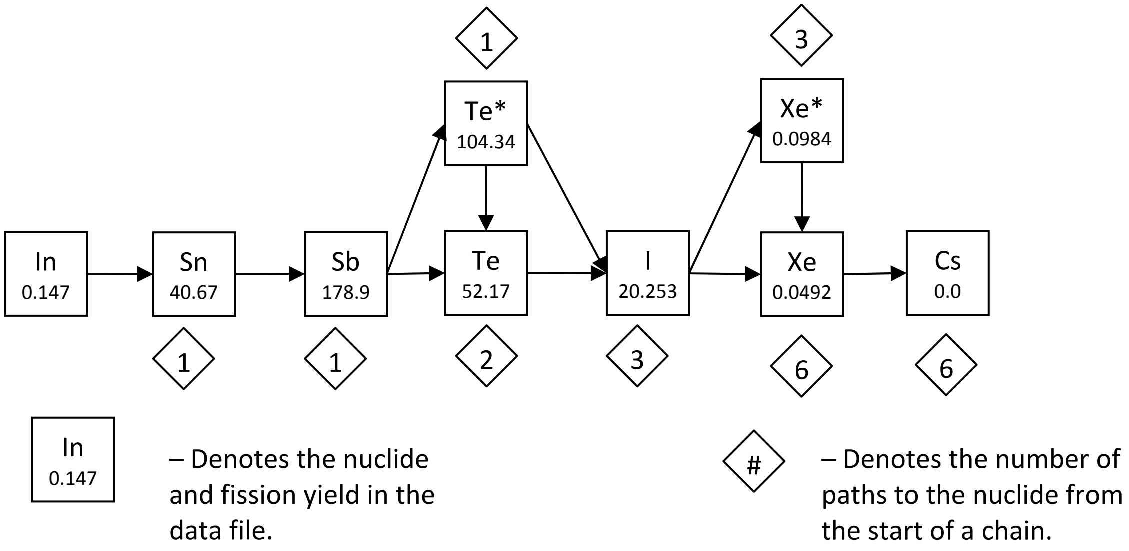
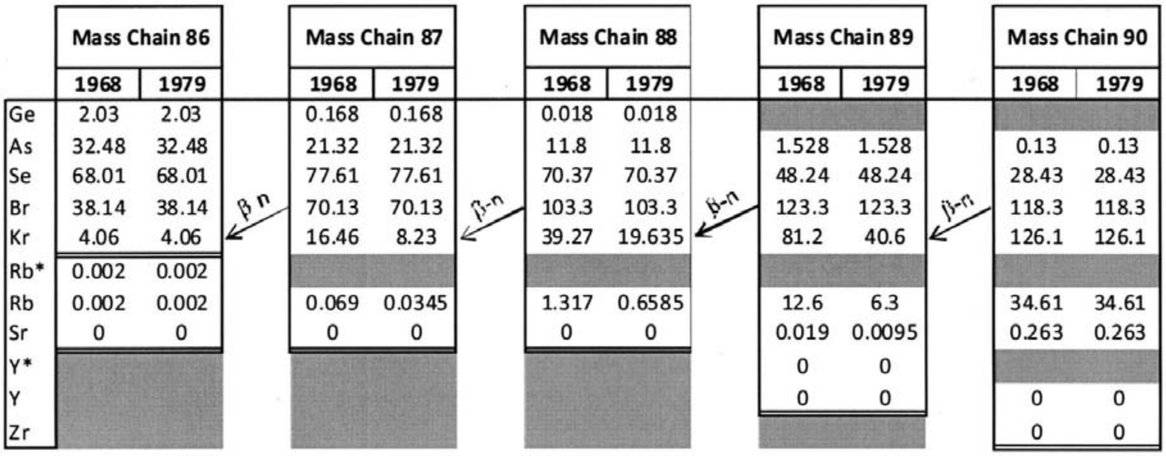


Fig. 3. 1979 fission yields for mass chain 133 (Norment 1979).

If the yields of each nuclide in the 1979 version are multiplied by the number of branches to that nuclide (the numbers in the diamonds), the resulting product is identical to the 1968 yields. This indicates a systematic modification of the yield values to account for branch merging. For example, ground state ^{133}Xe can be produced by decay in six different monolithic decay chains; the yield of ground state ^{133}Xe is divided equally among all six chains by assigning a one-sixth value of the true fission yield to each chain. Rather than handling this division within the code (as in the 1968 YIELD subroutine), the 1979 version anticipated the correction by dividing the yield value in the TAPE20 data by 6 and removing the YIELD subroutine.

The second case study is that of mass chains 86 through 90 (with fission yields shown for U238TN fission). In Fig. 4, b-n decay connects all five chains together and is most easily represented in tabular format.



	Mass Chain 86		Mass Chain 87		Mass Chain 88		Mass Chain 89		Mass Chain 90	
	1968	1979	1968	1979	1968	1979	1968	1979	1968	1979
Ge	2.03	2.03	0.168	0.168	0.018	0.018	▨	▨	▨	▨
As	32.48	32.48	21.32	21.32	11.8	11.8	1.528	1.528	0.13	0.13
Se	68.01	68.01	77.61	77.61	70.37	70.37	48.24	48.24	28.43	28.43
Br	38.14	38.14	70.13	70.13	103.3	103.3	123.3	123.3	118.3	118.3
Kr	4.06	4.06	16.46	8.23	39.27	19.635	81.2	40.6	126.1	126.1
Rb*	0.002	0.002	▨	▨	▨	▨	▨	▨	▨	▨
Rb	0.002	0.002	0.069	0.0345	1.317	0.6585	12.6	6.3	34.61	34.61
Sr	0	0	0	0	0	0	0.019	0.0095	0.263	0.263
Y*	▨	▨	▨	▨	▨	▨	0	0	▨	▨
Y	▨	▨	▨	▨	▨	▨	0	0	0	0
Zr	▨	▨	▨	▨	▨	▨	▨	▨	0	0

▨ - Denotes a nuclide that is not indexed in a particular mass chain.

- Denotes abundances for a stable nuclide.

Note: For mass number 86, two separate decay chains exist: Ge-Kr and Rb*-Sr. Also, for mass number 89, Y* is the parent of a one-decay chain to the common daughter Y.

Fig. 4. Comparison of fission yields for mass chains 86—90.

When b-n decay occurs, the daughter yield is reduced by an integer factor of the total number of branch merges preceding the daughter. Additionally, any subsequent decay daughters have modified yields. The most interesting case is that of mass chain 86, in which the stable daughter ^{86}Kr does not have its fission yield decremented. This would cause the initial inventory of ^{86}Kr to be twice its real value and would therefore violate conservation laws. However, the exposure and activity calculations would remain unaffected because there is no decay from ^{86}Kr.

1.3.4 1992 Treatment of Branch Merging—BATMAN Correction

In the 1992 revision of DELFIC, the subroutine BATMAN was modified using a unique method intended to preserve conservation (Roberts et al. 1992). First, for each mass chain, the fission yields were modified in a manner similar to YIELD in 1968. An algorithm was then added to determine which nuclides were affected by branch merging after b-n decay. The yields for those particular nuclides were then assigned to only one of the monolithic chains they inhabited. In this manner, the presumed redundancy of the post-merge nuclides was removed.

Unfortunately, although the BATMAN subroutine was modified to correct for branch merging, the data file containing the fission yields (TAPE20.DAT) remained identical to the 1979 ABEGN data file. Therefore, the fission yields were adjusted once in the data file in 1979, then a second time in the subroutine in 1992. This had the effect of underpopulating the yields for the affected nuclides.

The reason for this discrepancy appears to be a lack of a discussion that explains the modification to TAPE20.DAT between the 1968 and 1979 versions of DELFIC. The removal of the YIELD subroutine and the adjustments to the fission yields in ABEGN do not seem to be documented. When investigating the 1979 version, the 1992 team likely never noticed the changes to the fission yields in the data files and assumed that the adjustment for branch merging had never been applied.

1.3.5 Branch Merging Summary

In the 1968, 1979, and 1992 versions of DELFIC, three different approaches were used to account for branch merging. A problem does occur in the SAIC code because the 1992 correction was applied with the modified 1979 fission yields still in place. In any version of DELFIC, particular care should be taken to ensure that branch merging is corrected only once, given the problematic history of branch merging in the revision process.

1.4 NUCLIDE DESCRIPTION (NUCLID AND BREAKUP.DAT)

1.4.1 1968 and 1979

In 1968, the original programmers of DELFIC devised an octal coding system to store information about each nuclide. In this system, each nuclide could be uniquely identified by its nuclear composition and its decay patterns. The octal code was used to store each nuclide's mass number, atomic number, isomeric state, number of decay modes, and information regarding the daughter of decay. All of the coded information for each nuclide was concatenated to form a single coded word of 12 octal digits. In the 1968 and 1979 versions of DELFIC, these words were stored in the PAM1 subroutine under the data heading NUCLID. The coding of each piece of information and the assembly of the final word are shown here using the first fission product in NUCLID in these versions of DELFIC: Cobalt 72.

1.4.1.1 Nuclear composition

Mass Number—The mass number was stored in the first three octal digits. The number was simply the octal equivalent of the mass number. For ^{72}Co, the octal equivalent of 72 is 110 ($64*\underline{1} + 8*\underline{1} + 1*\underline{0}$).

Atomic Number—The atomic number was stored in the next three octal digits. For ^{72}Co, the octal equivalent of the atomic number (27) is 033 ($64*\underline{0} + 8*\underline{3} + 1*\underline{3}$).

Isomer—The isomeric state was stored in one octal digit. For ground state nuclides, the isomer value was 0. If the nuclide was metastable, the isomer digit would be a 1 or 2. For most metastable isomers, the value was 1; for nuclides with multiple metastable isomeric states, one isomer was assigned the value of 2. Since ^{72}Co is in the ground state, its isomer digit equals 0.

1.4.1.2 Decay information

The coding of decay information for a nuclide was dependent on the order in which nuclides were stored in the data list NUCLID. The nuclides were ordered by mass chain (lightest to heaviest), then by atomic number (fewest number of protons to greatest), then by isomeric state (most energetic metastable state to ground state). Rather than store the type(s) of decay for each nuclide (e.g., beta decay, IT, etc.), DELFIC stored the distance between parents and daughters in the list. In this system, decay information could be stored purely by numeric values representing the distance (the "increment"), whether the daughter was listed before or after the parent, and how many possible daughters existed for each nuclide.

Daughter Increments—DELFIC could store information for up to three modes of decay for each nuclide. For each decay mode, the magnitude of increment between the parent and each daughter was stored in a single octal digit (for a total of three octal digits). The increments for all three decays are stored in concatenated digits so that the first decay increment is in the leftmost octal digit, the second decay increment (if it exists) is in the central octal digit, and the third decay increment (if it exists) is in the rightmost octal digit. For ^{72}Co, the only mode of decay is beta decay. The daughter (^{72}Ni) was listed in NUCLID in the position directly below ^{72}Co, so the increment was a 1. Therefore, the coded daughter increments for ^{72}Co are 1 0 0. The zeroes for decay modes 2 and 3 indicate that ^{72}Co does not have a second (or third) decay mode. A stable nuclide consists of zeros across all digits.

The daughter increment digits store the magnitude of increment but not whether the increment is positive (i.e., the daughter is below the parent in NUCLID) or negative (i.e., the daughter is above the parent in NUCLID). A nuclide with a single electron capture as a decay would have identical daughter increments to ^{72}Co (assuming the daughter of electron capture is listed immediately prior to the parent).

Direction—The daughter increments described only the magnitude of the distance between the parent and daughter(s) in the index. The direction increment informed DELFIC whether the daughter was found above the parent in the nuclide list (a “negative” increment) or below the parent in the nuclide list (a “positive” increment). Because of the list order in NUCLID, the daughters of isomeric transitions and beta decays are always found below the parent and have a positive increment. For positron, electron capture, b-n, and alpha decays, the increments from the parent to the daughter are negative.

The direction octal digit was allowed one of four values: 4, 3, 2, and 0. A “4” indicated that the increment of the first branch was negative; a “3” indicated that the increment of the second branch was negative; a “2” indicated that the increment of the third branch was negative; and a “0” indicated that no branch had a negative increment. For ^{72}Co, the single mode of decay has a positive increment, so the value of the direction digit was 0. With this convention, only one of the three possible decay modes for each nuclide could be negative.

Branching—The final octal digit stored the number of decays available to a nuclide. The coding used for the branching digit was similar to that for the direction digit. If the nuclide was stable or had one decay mode, the branching octal digit would equal 4 (in binary form, the leftmost bit would be a 1). If the nuclide had two decay modes, the branching octal digit would equal 2 (in binary, the middle bit would be a 1). If three decay modes were available, the branching octal digit would equal 1 (in binary, the rightmost bit would be a 1). If the nuclide was stable, the branching digit was assigned a value of 4.

In all cases, a binary 1 would appear exactly once in the branching digit. The “1” bit inhabited the same relative position in the branching bits that the final decay mode inhabited in the octal digits of the daughter increments. For example, ^{72}Co has one mode of decay. The daughter increments—in octal form—are represented as 1 0 0. The branching digit for ^{72}Co equals 4 in octal form, which is 1 0 0 in binary form. The “1” in the branching bits inhabits the leftmost binary position, indicating that the final increment exists in the leftmost octal digit in the daughter increments. Since the decay modes are listed from left to right, this indicates that only one decay mode exists for ^{72}Co.

To conserve memory, all of the above information was concatenated into a single word in NUCLIDE. This word was the decimal equivalent of the 12 consecutive octal digits shown in Fig. 5.

For ^{72}Co, the octal values are shown in Fig. 6.

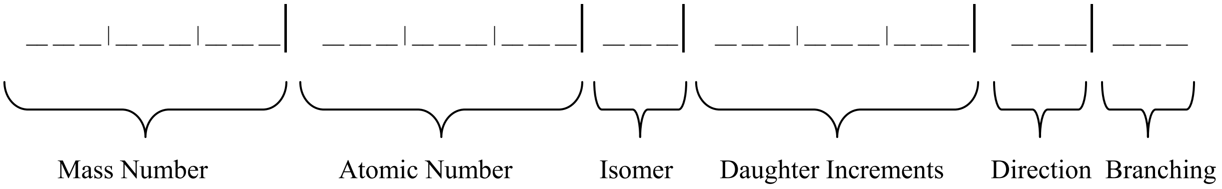


Fig. 5. Binary description of NUCLID.

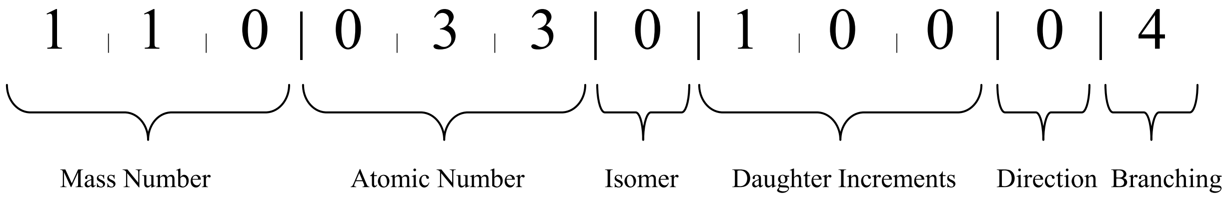


Fig. 6. Concatenated octal code for ^{72}Co.

This concatenated code was then converted to decimal form for storage in NUCLID. For ^{72}Co, the value of the octal code was 9670758404. Since ^{72}Co was the beginning of a decay chain in DELFIC's fission product library, a negative sign was attached to the NUCLID value, resulting in a value in NUCLID of –9670758404. In this system, DELFIC required only a maximum of 11 decimal digits to store the nuclear composition and data for up to three decay modes for a particular nuclide.

Since all nuclide information in NUCLID was stored in octal form, the information could very easily be extracted through the use of INT and MOD functions. For example, MOD (9670758404,8^9) equals 72, the mass number for ^{72}Co. Also, MOD (INT(9670758404/8^9),8^6) equals 27, the atomic number for ^{72}Co.

1.4.2 Limitations

Using an octal coding system enabled DELFIC to efficiently discern nuclide information from a very compact data value. Yet the system did have some limitations due to the manner in which the coded values were generated and concatenated. The following limitations did not affect the decay chains in the original list of DELFIC nuclides, but they did present an obstacle to any attempt to upgrade the nuclide list as information about fission products increased. These limitations are the most likely reasons that the nuclide inventory in DELFIC was never upgraded from the original 700 nuclides, even though the original list was developed 40 years ago.

Negative Increments—The logic in DELFIC did not allow for multiple negative decay increments (e.g., electron capture to both an excited state and a ground state). In the subroutine BATMAN (and in YIELD in 1968), the variable "IM" was used as a placeholder to identify which decay branch of a nuclide was included in a given monolithic chain. IM was initialized to equal 4 for the first branch, then decremented by 1 for each subsequent branch through the various monolithic chains of decay. To determine if the increment of a nuclide to its daughter was negative, the value of IM was compared with the value of the direction increment. If the two values were equal, the increment was negative.

With this system, an exact match was required between the Direction increment and the variable IM to label an increment as negative. Because of the need for an exact match, the Direction increment could provide information for only one negative increment per nuclide. For example, if the first branch of a nuclide represented b-n decay, the Direction digit would equal 4. If that same nuclide also had a probability of electron capture, DELFIC could not correctly store that decay information; electron capture would require a negative increment, but the Direction digit was already reserved by the b-n decay.

In the original list of 692 fission product nuclides, electron captures were rare, b-n decays were sparse, and alpha decays did not exist. In all likelihood, the 1968 DELFIC team had no indication that any of the 692 nuclides should have multiple negative increments, so this potential limitation probably never affected the decay logic. However, upgrading the nuclide and decay inventory would necessarily require more nuclides and more decays with negative increments. Removing this logical limit made it possible to accurately model far more complicated decay patterns.

Magnitude of Increments—Each daughter increment was stored in a single octal digit. With this space limitation, no daughter increment could be greater than a distance of 7 (represented as 111 in binary) from the parent nuclide. In some instances of b-n decay, increments of up to 7 were used; it is assumed that the decay chain data in 1968 naturally fit this limitation so that no decay data were lost.

This limitation prevented the inclusion of alpha decay, however, as the incremental distances would have been much larger. Fortunately, alpha decays among fission products are very rare and were possibly not yet known to the original DELFIC programmers. However, a newer nuclide inventory—with more nuclides and more complete decay information—would likely have b-n decays with increments greater than 7 and would likely have information for alpha decays with even larger increments. To accommodate this possibility, the coding and storage system would have to be upgraded to handle increments greater than 7 in magnitude.

Machine Word Limits—The final note that Tompkins (1968) provides in his documentation notes that some machines may not be able to fulfill the 36 bit (12 octal digits) word length requirement. In this case, he noted that the number could be effectively split between the isomer digit and the daughter increment digits to create two arrays of 21 bit and 15 bit words, respectively. This very concept became a part of the revision of DELFIC in 1992.

1.4.3 1992

Part of the work performed on DELFIC by SAIC included the restoration of an electronic version of the code. When SAIC generated the electronic code, it followed Tompkins' advice to split the NUCLID word. Since memory was no longer the dramatic restriction on data storage that it had been in the 1960s, SAIC broke the word apart into several arrays in a file labeled BREAKUP.DAT (Fig. 7).

Index	masstab	nattab	nuclida	nuclidb	nuclidc

Fig. 7. Layout of the NUCLID data in SAIC's BREAKUP.DAT.

As an example, the generation of the values for ^{72}Co is illustrated in Table 1.

Table 1. Description of BREAKUP.DAT

	Number	How calculated
1968 NUCLID	–9670758404	
Mass number (A)	72	$=\mathrm{INT}(\lvert\mathrm{NUCLID}\rvert/8^{9})$
Atomic number (Z)	27	$=\mathrm{INT}(\mathrm{MOD}(\lvert\mathrm{NUCLID}\rvert,8^{9})/8^{6})$
Nuclide index	–36891	$=\mathrm{SIGN}(\mathrm{NUCLID})*\mathrm{INT}(\lvert\mathrm{NUCLID}\rvert/8^{6})$
Daughter index	4100	$=\mathrm{MOD}(\lvert\mathrm{NUCLID}\rvert,8^{5})$
Branching index	4	$=\mathrm{MOD}(\lvert\mathrm{NUCLID}\rvert,8^{1})$

i	masstab	nattab	nuclida	nuclidb	nuclidc
1	72	27	–36891	4100	4

Index—The index number was an integer that stated the position in the array for the line of data.

Masstab—The masstab number was a decimal number and was the mass number of the nuclide.

Nattab—The nattab number was the atomic number of the nuclide in decimal form.

Nuclida—The nuclida number was the decimal representation of the leftmost six octal digits in the original NUCLID value. In other words, SAIC generated nuclida by separating the mass number and atomic number digits from NUCLID and creating a new numeric scheme—very similar to the concept proposed by Tompkins (1968). This value appears redundant when it is placed alongside the masstab and nattab numbers, but it allowed for minimal modification of the DELFIC code. Additionally, the negative sign that indicated the beginning of a decay chain was included in the nuclida word.

Nuclidb—The nuclidb number was composed of the rightmost five octal digits of the original NUCLID word. This contained the decay information for each nuclide in the same manner as the previous editions of the code. Because the logic of the decay coding was unchanged, the limitations on negative increments and magnitudes of increments still applied.

The original list of 692 nuclides did not require many different values of nuclidb to describe all of the increments used in decay. Table 2 provides a list of all values of nuclidb for this data set, along with the physical decays that are most commonly associated with the values and the sequence of daughter increments. Note that the physical decays described in the table are only the most common types for a given number; the coding is designed to describe the increment to the daughter(s), not to describe the actually decay mode. For example, “4100” may represent either beta decay or isomeric transition.

Table 2. nuclidb values for the original DELFIC nuclides

nuclidb	nuclidb (octal digits)	Daughter increments	Number of occurrences	Common decay patterns
4	000|0|4	None—Stable	108	Stable
4100	100|0|4	+1	498	β^-
4642	110|4|2	–1, +1	1	ε, IT
5122	120|0|2	+1, +2	47	IT, β^-
5154	120|4|2	–1, +2	1	ε, β^-
5313	123|0|1	+1, +2, +3	3	IT, β^-, β^-
5761	132|0|1	+1, +3, +2	1	IT, β^-, β^-
8196	200|0|4	+2	20	β^-
8738	210|4|2	–2, +1	2	ε, β^-
12292	300|0|4	+3	4	β^-
21026	510|4|2	–5, +1	2	n, β^-
25122	610|4|2	–6, +1	3	n, β^-
29218	710|4|2	–7, +1	2	n, β^-

Nuclidc—The nuclidc number was created from the final octal digit in the NUCLID word. Technically, creation of this number was redundant, as the branching information was contained in the nuclidb number. The primary reason for the explicit generation of this number appeared to be convenience, particularly for the algorithm generated by SAIC to detect branch merging.

1.4.4 Comments

In generating the BREAKUP.DAT file, SAIC eliminated the octal digit that stored the isomeric state of each nuclide (the digit referred to as "Isomer" previously). The digit was likely eliminated because DELFIC never used the information in the coding. The information of this digit was implicit in the order in which the nuclides are stored in BREAKUP.DAT (and previously in NUCLID); isomeric states were listed prior to the ground states in the arrays.

In order to facilitate the interpretation of the information contained in the NUCLID words, DELFIC contained a list of powers of 8, from 8^1 to 8^{11}. This list has been noted to provide compiling errors in the electronic version of the 1979 code, as the 8^{11} exceeds the maximum length of an INTEGER*4 type in FORTRAN. However, this number was never used in the original or the SAIC version of the code.

In the report for the 1992 upgrade (Roberts et al. 1992), SAIC incorrectly described the capabilities of DELFIC's decay logic. In Sect. 2, the decay is listed as "limited to beta decay, beta-neutron decay and isomeric transition (IT)." The error is reinforced later at the end of Sect. 2: "At this time nothing has been done to include additional decay modes, such as positron emission or electron capture, in the DELFIC decay scheme…" In fact, the decay logic was perfectly suited to handling positron emission or electron capture through the use of negative increments (much like the process used to handle b-n decay). Additionally, the original NUCLID data and SAIC's BREAKUP.DAT file actually *included* electron capture decay events. In the original list of 692 nuclides, the nuclides with electron capture decay are ^{122}Sb, ^{128}I, and ^{152}Eu (ground and excited states). As mentioned before, DELFIC's logic could have readily accounted for the negative increments of alpha decay if the daughter were located within seven increments of the parent.

The perceived limitation mentioned by Roberts et al. (1992) was partly based on the misinterpretation of a very real limitation in the decay logic—the inability to have more than one negative increment (e.g., both electron capture and b-n decay branches) from a single parent as a result of the limitations on the Direction octal digit (nuclidb in the 1992 version). As Roberts et al. correctly noted, DELFIC would not likely be able to handle an upgrade in the nuclide inventory without improving the decay logic. But the limitation was not an inability to handle these decays; the limitation was an inability to handle multiple occurrences of these decays for a single parent.

1.5 COMPARISON OF YIELD DATA FILES (TAPE20.DAT)

1.5.1 Cumulative Fission Yields

In DELFIC, the fission yields are handled in units of [atoms/10,000 fissions]. These nonstandard units were likely chosen to contain the exponents between +3 and −3, reducing the number of bytes required to save the yields. (In the computer coding practices of the 1960s and 1970s, this technique was routine since memory space was much more valuable than today.) Additionally, the assumption was implicit that only two fission fragments were produced per fission; there are no yield data for the smaller fragments of ternary fission. Therefore, all fission yields for a given fission should sum to 20,000 in DELFIC units if the yield data are unadjusted. Adjusted yield data would have a reduced cumulative yield as a result of the correction for branch merging discussed earlier in this report.

The 1968 yields are not currently stored in electronic fashion, and summing the yields of a particular fission is a somewhat tedious affair. But comparing the 1968 and 1979 cumulative yields for thermonuclear fission of ^{238}U (U238TN) reveals the difference in Table 3.

Table 3. Comparison of total U238TN yields for 1968 and 1979 data

1968	19917.58	(atoms/10,000 fissions)
1979	19493.84	
Difference	423.74 (2.13%)	

Summing the yields for a particular fission type also provides one check for the reasonability of the yield: if the yields do not sum to 20,000 (within a reasonable margin of error), they are suspect and perhaps unusable. In the 1968 version, for example, the U238TN yield is 0.4% below the 20,000 atoms per fission total. Given the degree of round-off applied to the yields in the 1968 data, this is a reasonably close account of the fission yield.

The electronic versions of the 1979 and 1992 yields are identical and may be summed much more readily. For all 12 fission types, the cumulative yields are given in Table 4.

Table 4. Total fission yields on TAPE20.DAT

Cumulative fission yields (atoms per 10,000 fissions)	
Fission type	**TAPE20.DAT**
P239FI	18981.40
P239HE	18793.03
P239TH	19327.66
U233FI	18490.73
U233HE	18274.42
U233TH	18792.36
U235FI	18983.79
U235HE	19678.16
U235TH	19275.64
U238FI	20363.16
U238HE	19662.05
U238TN	19493.84

The TAPE20 yields sum closely to 20,000, although most yields are noticeably deficient. Most of the deficiencies in the TAPE20 yields appear to be largely explainable by the correction for branch merging. The most notable cumulative yield is that for U238FI in TAPE20, which is greater than 20,000 despite being corrected for branch merging.

There is a risk in importing an external fission yield, such as the yield in ORIGEN, into DELFIC. The DELFIC program is currently designed to handle an inventory of 700 nuclides. (The 700 nuclides were defined in the 1979 DELFIC by the array NUCLID and in the 1992 DELFIC by the array nuclidb. All fission types were constrained to yields of only those nuclides. This list of nuclides was unchanged since the original version of DELFIC.) If those 700 nuclides are simply extracted from a modern yield library with many more nuclides and substituted into DELFIC's existing dataset, conservation of the fission fragments will be lost and the inventory of fallout nuclides may have a considerable shortfall. Adaptation of an external fission yield set to DELFIC required an extensive revision of DELFIC's logic and NUCLID data to accommodate the new decay chains.

2. UPGRADES AND MODERNIZATION

2.1 INTRODUCTION

Initially, DELFIC allowed for a maximum of 700 fission products, either by immediate production or by subsequent decay of fission products. In practice, DELFIC has always used a list of 692 nuclides with atomic numbers ranging from 27 to 66 and mass numbers ranging from 72 to 161. While this list was mostly comprehensive of nuclides produced by fission, it had not been updated since DELFIC's original creation. In contrast, modern fission yields—such as those used in ORIGEN—contain up to roughly 1100 nuclides. Additionally, the decay modes of the fission products were effectively 40 years out of date. The decay constants were updated in 1992, but the branching ratios have never been updated. For this reason, updating the nuclide database and ensuring DELFIC's ability to process such a database were the primary goals of this upgrade.

To update the fission yields and decay data, the ENDF/B-VII data in ORIGEN were used. A FORTRAN program was constructed to read the card images and to produce the BLOCKB.FOR (also known as PAMDAT1), TAPE2008.DAT, and BREAKUP2008.DAT files. The TAPE2008.DAT file contains unmodified fission yields rather than modified yields as found in the 1979 and 1992 versions of DELFIC. To correctly account for branch merging, an adapted version of the YIELD subroutine from the 1968 DELFIC code was added to DELFIC. The new YIELD subroutine would then modify the yields within the program to account for branch merging, but the data files would be left intact.

This section discusses the changes made in the DELFIC code, along with the rationale for each change. The changes in the data files are discussed in a similar manner. In brief, the modifications are

- replacement of the original DELFIC fission yields with unmodified fission yields from the ORIGEN-S library (based on ENDF/B-VII),
- expansion of the fission yield library to include fission types for 30 actinide isotopes,
- revision of the exposure rate multiplier (ERM) data with new multipliers that account for the new fission yields and photon yields, and
- expansion of the decay chain logic to accommodate more complex decay modes contained in ORIGEN.

2.2 FISSION YIELD VERIFICATION AND UPGRADE

2.2.1 Comparison of DELFIC to ORIGEN

As a check of the original fission yields of DELFIC, the 1979 DELFIC decay engine was tested against ORIGEN. To accomplish this, the DELFIC branching ratios and decay constants were converted into an ORIGEN-formatted card-image input deck. The yields of a 10,000-fission event were then introduced to both ORIGEN and DELFIC, and the outputs were compared for various times and mass chains. The mass chains were selected to test different levels of complexity of the decay chains, and the decay times were selected by considering the half-lives of the observed nuclides and evaluating the decays at various stages of the decay process.

Since DELFIC is primarily interested in activity and exposure calculations, the output had to be modified to determine the nuclide abundances at a given time. Map Option 3 (exposure rate at time H + T1 hours) was selected, with T1 chosen to allow a reasonable amount of decay within the chain. The activities of each nuclide were printed by setting NPRNT(9) to true, and each nuclide's activity was then divided by the nuclide's decay constant to determine the abundance of each nuclide. A 1 kt yield was selected, although this is a formality as the outputs are normalized to a per-10,000-fission yield. The end result was to calculate the number of atoms of each nuclide at the given time T1 after a 10,000 fission event.

In ORIGEN, the initial inventories of the observed mass chains were directly input into the ORIGEN-ARP interface. Then the nuclides were allowed to decay for a specified time and the final abundances were compared against the DELFIC abundances. It should be noted that the initial yields given to ORIGEN-ARP were the numerical values of the 1968 yields, whereas the modified 1979 yields were used in the 1979 version of DELFIC. Using the 1968 data gave ORIGEN the true yields rather than the modified yields, and using gram-atoms allowed for a direct numerical comparison of the decay by numbers of atoms rather than by mass. By using the unmodified yield values in ORIGEN, the end result was to calculate the number of atoms of each nuclide at a given time after a 10,000 fission event. This allowed for a direct comparison between the 1979 DELFIC and ORIGEN decay outputs, shown in Table 5 through Table 9.

Table 5. Mass chain 92 after 1 min of decay

Simple Decay Chain - Betas only, no metastables			U-235th Yield	$t_{1/2}$	**DELFIC Output**	**ORIGEN Output**
A	Z	Element	(atoms/10^4 fiss)	(sec)	Time = 1 minute	
92	34	Se	0.00E+00	0.01	1.000E-34	0.000E+00
92	35	Br	5.39E+01	1.5	4.902E-11	4.902E-11
92	36	Kr	2.31E+02	3	3.231E-04	3.231E-04
92	37	Rb	2.46E+02	5.3	3.713E-01	3.712E-01
92	38	Sr	6.59E+01	9720	5.943E+02	5.943E+02
92	39	Y	6.05E-01	12960	2.764E+00	2.766E+00
92	40	Zr	0.00E+00	Stable		4.974E-03

Table 6. Mass chain 150 after 1 s of decay

Simple Decay Chain - Betas only, no metastables			U-235th Yield	$t_{1/2}$	**DELFIC Output**	**ORIGEN Output**
A	Z	Element	(atoms/10^4 fiss)	(sec)	Time = 1 second	
150	56	Ba	0	0.01	0.000E+00	0.000E+00
150	57	La	8.35E-01	1.5	5.260E-01	5.260E+00
150	58	Ce	1.35E+01	2.5	1.050E+00	1.050E+01
150	59	Pr	3.02E+01	15	3.207E+01	3.207E+01
150	60	Nd	1.70E+01	Stable		1.844E+01

Table 7. Mass chain 133 after 1 min of decay

Beta Decay Chain with metastables			U-238tn Yield	$t_{1/2}$	**DELFIC Output**	**ORIGEN Output**
A	Z	Element	(atoms/10^4 fiss)	(sec)	Time = 1 minute	
133	49	In	0.14700	0.01	0.000E+00	0.000E+00
133	50	Sn	4.0670E+01	39	1.405E+01	1.405E+01
133	51	Sb	1.7890E+02	158.4	1.606E+02	1.606E+02
133	52*	Te	1.0434E+02	3000	1.351E+02	1.351E+02
133	52	Te	1.0434E+02	750	1.112E+02	1.112E+02
133	53	I	6.0760E+01	74880	6.816E+01	6.816E+01
133	54*	Xe	2.9530E-01	198720	2.961E-01	2.961E-01
133	54	Xe	2.9530E-01	455328	3.302E-01	3.302E-01
133	55	Cs	0.00E+00	Stable		2.854E-05

Table 8. Mass chain 133 after 10 min of decay

Beta Decay Chain with metastables			U-238tn Yield	$t_{1/2}$	**DELFIC Output**	**ORIGEN Output**
A	Z	Element	(atoms/10^4 fiss)	(sec)	Time = 10 minutes	
133	49	In	0.14700	0.01	0.000E+00	0.000E+00
133	50	Sn	4.0670E+01	39	9.541E-04	9.541E-04
133	51	Sb	1.7890E+02	158.4	1.687E+01	1.687E+01
133	52*	Te	1.0434E+02	3000	2.238E+02	2.238E+02
133	52	Te	1.0434E+02	750	1.019E+02	1.019E+02
133	53	I	6.0760E+01	74880	1.460E+02	1.461E+02
133	54*	Xe	2.9530E-01	198720	3.084E-01	3.084E-01
133	54	Xe	2.9530E-01	455328	8.521E-01	8.521E-01
133	55	Cs	0.00E+00	Stable		0.000E+00

Table 9. Mass chains 86–90 after 1 min of decay

B-n decay chains			U-238tn Yield	$t_{1/2}$	**DELFIC Output**	**ORIGEN Output**
A	Z	Element	(atoms/10^4 fiss)	(sec)	Time = 1 minute	
86	32	Ge	2.030E+00	0.01	0.000E+00	0.000E+00
86	33	As	3.248E+01	2	3.215E-08	3.215E-08
86	34	Se	6.801E+01	16	7.986E+00	7.986E+00
86	35	Br	3.814E+01	60	7.889E+01	7.889E+01
86	36	Kr	4.060E+00	Stable	╳	6.006E+01
87	32	Ge	1.680E-01	0.01	0.000E+00	0.000E+00
87	33	As	2.132E+01	1.5	1.954E-11	1.954E-11
87	34	Se	7.761E+01	16	7.531E+00	7.531E+00
87	35	Br	7.013E+01	54.5	8.784E+01	8.784E+01
87	36	Kr	1.646E+01	4680	9.946E+01	9.946E+01
87	37	Rb	6.900E-02	6.93E+14	5.984E-01	5.985E-01
87	38	Sr	0.000E+00	Stable	╳	5.354E-14
88	32	Ge	1.800E-02	0.01	0.000E+00	0.000E+00
88	33	As	1.180E+01	0.01	1.470E-13	0.000E+00
88	34	Se	7.037E+01	2.5	4.900E-06	4.901E-06
88	35	Br	1.033E+02	16.3	1.502E+01	1.502E+01
88	36	Kr	3.927E+01	10080	2.170E+02	2.170E+02
88	37	Rb	1.317E+00	1080	1.929E+00	1.929E+00
88	38	Sr	0.000E+00	Stable	╳	6.043E-02
89	33	As	1.528E+00	0.01	0.000E+00	0.000E+00
89	34	Se	4.824E+01	2	4.635E-08	4.635E-08
89	35	Br	1.233E+02	4.4	1.685E-02	1.685E-02
89	36	Kr	8.120E+01	192	2.094E+02	2.094E+02
89	37	Rb	1.260E+01	924	5.747E+01	5.747E+01
89	38	Sr	1.900E-02	4363200	1.570E+00	1.570E+00
89	39*	Y*	0.000E+00	16	╳	0.000E+00
89	39	Y	0.000E+00	Stable	╳	5.896E-06
90	33	As	1.300E-01	0.01	0.000E+00	0.000E+00
90	34	Se	2.843E+01	0.01	1.060E-12	0.000E+00
90	35	Br	1.183E+02	1.6	7.550E-10	7.550E-10
90	36	Kr	1.261E+02	33	7.297E+01	7.296E+01
90	37	Rb	3.461E+01	162	1.801E+02	1.801E+02
90	38	Sr	2.630E-01	883612800	3.271E+01	3.271E+01
90	39	Y	0.000E+00	231465.6	6.060E-07	6.302E-07
90	40	Zr	0.000E+00	Stable	╳	3.300E-11

From Table 5 to Table 9, it can readily be seen that DELFIC and ORIGEN produce very similar decay results, given the same initial inventories and modes of decay. In the DELFIC output, the stable nuclides are not given values because the DELFIC code does not keep track of stable nuclide inventories. The most significant discrepancy between the DELFIC and ORIGEN results was the inventory of ^{90}Y in Table 9. Here, DELFIC calculated 6.060E–07 atoms/10^4 fissions whereas ORIGEN calculated 6.302E–07 atoms/10^4 fissions. However, this is a true difference of about 3E–08 atoms for every 10,000 fissions and is well within a reasonable computation margin of error given the sizes of the inventories of the preceding nuclides in the decay chain.

The agreement of results indicates that the 1979 DELFIC fission yields and decay calculator did indeed account for branch merging correctly. The added step in the 1992 DELFIC (zeroing out the yield value after the first application) was therefore unnecessary and resulted in a loss of conservation. Again, the 1992 revision was most likely introduced as a result of a lack of cogent documentation regarding the modification of the fission yield data in the 1979 version.

2.2.2 Generation of BLOCKB.FOR

In 1992, SAIC moved much of the nuclear data in DELFIC from the PAM1 subroutine to a data file called BLOCKB.FOR. The information in this file included the branching ratios, decay constants, ERMs, induced soil activity data, and various reference numbers. Given the current improvement in the fission yield data and the nuclide inventory, much of the data in PAMDAT1 had to be replaced. The replacement was performed automatically in the data conversion program by reading the ORIGEN-S data libraries. With the more complex decay modes, the number of branching ratio values increased from 128 to 778. The ERM database was upgraded to include all ERM values calculated by SAIC in 1992 plus the ERM values for nuclides not originally listed in DELFIC.

The induced soil activity data did not depend on the nuclide data and were left untouched because of time constraints. Since an ERM value was listed for every nuclide, the JRM data were removed and the subroutine GXPSR was modified to anticipate an ERM value for every nuclide rather than a select list. The final MULT value (8^11) was removed as a matter of compiler convenience; the value exceeded the INTEGER*4 limit and caused warnings during compiling. This MULT value was never used in the program (even the 1968 version) and was therefore unnecessary.

2.2.3 Generation of the New Fission Yields

ORIGEN-S contains fission yield data for 90 unique fission types—high-energy neutron, fission neutron, and thermal neutron-induced fission yields for 30 isotopes. As a part of the upgrade, the data conversion program read the card images of the fission product libraries of ORIGEN-S and formatted the yields into DELFIC form. The units of the yields were converted to DELFIC's standard of atoms per 10,000 fissions. For convenience, the 12 fission types originally found in DELFIC were listed first in the new TAPE2008.DAT data file.

The use of the ORIGEN-S libraries provided several advantages over the previous yields. First, since the ORIGEN yields are based directly on the ENDF/B-VII database, they contain the most recent and comprehensive yield data available. The new list contains 1096 nuclides, compared with the original 692 nuclides in DELFIC. Second, the new yields more consistently match the theoretical 20,000 fission products per 10,000 fissions (assuming exactly 2 fission products per fission) than the original yields, which tended to underestimate the number of fission products (see Table 4). Third, the new yields contain data for ternary fissions, which include basic yields for hydrogen and helium production.

It should be noted that ORIGEN-S does not inherently contain fission yields for thermonuclear (TN) neutron spectra. Instead, ORIGEN-S includes thermal-neutron fission yields for fissionable isotopes (^{238}U, ^{238}Pu, etc.) that are identical to the fission-neutron fission yields for those isotopes. To provide thermonuclear yields for the fissionable isotopes, the method used to generate the original DELFIC U238TN yield was investigated and adopted (Crocker 1963).

Crocker made use of studies on the two-mode fission hypothesis (Levy et al. 1961) to assert, in effect, that for any incident neutron energy, the yield of any fission product for a fissionable isotope may be estimated by linear interpolation of changes in that fission product's yield as a function of incident neutron energy. In fact, Crocker used the fission yields of 28 isotopes from a Health and Safety Laboratory study (Hallden et al. 1961) to identify the approximate location of the ^{238}U thermonuclear fission yield; then, according to Crocker, "A smooth curve was drawn through the outline provided by the points thus obtained. The curve was then normalized to yield 200 fragments for 100 U-238 fissions." Crocker chose to sketch his curve around an axis of symmetry that corresponded to "the prompt emission of 3 neutrons per fission" (Crocker 1963). Using the criterion of three prompt neutrons per fission from Crocker, a U238TN yield from the U238FI and U238HE yields can be generated by interpolating between the two yields and using a weighting of 92.1% U238FI and 7.9% U238HE (Fig. 8).

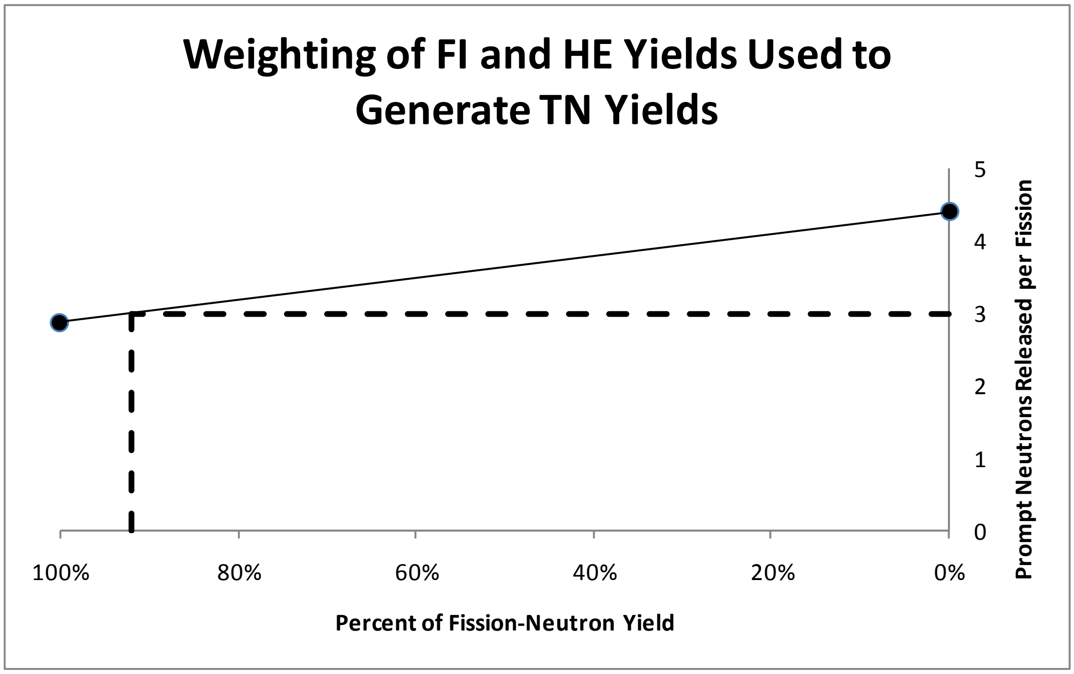


Fig. 8. Generating the TN yield based on the number of prompt neutrons released.

With Crocker's example as a guide, the fission yields of the fission-neutron and high-energy-neutron fissions of fissionable isotopes were weighted to provide a convenient and reasonable number of neutrons per fission. Yields could be interpolated for every single fission product with the ORIGEN-S data, so no hand-sketching of the fission yield curve was necessary. The same weighting scheme was used for all thermonuclear spectra. The weighting was skewed more heavily toward the fission-neutron energies, and the weighting for ^{238}U was chosen to match the same number of neutrons per fission that Crocker used in the 1968 version of DELFIC.

For all fissionable fuels, the thermonuclear-neutron yields for each fission product were generated with Fig. 8.

$$Nuclide\ Yield_{,TN} = 0.921 * Nuclide\ Yield_{,FI} + 0.079 * Nuclide\ Yield_{,HE}$$

Equation 1. Weighting system used to generate TN yields.

The weighting factors for the FI and HE yield values were chosen to generate the same number of neutrons per fission for U238TN as was used in Crocker's original U238TN yields for DELFIC. This ratio was then applied to all fissionable fuels to provide a consistent method for generating the thermonuclear fission yields. Without any stronger rationale for choosing a yield generation scheme, this method provided consistency with Crocker's yields and provides yields that should be sufficient for modeling explosions where the neutron energies are rather dependent on weapon composition. As was noted by Crocker: "It should be borne in mind that the neutron energy spectrum of a thermonuclear explosion is not well-defined, but varies from one explosion to another. Variations as large as a factor of two greater or smaller than the estimated yields would not be unexpected in the sensitive regions of the curve" (Crocker 1963). An illustration of the new U238TN fission yield can be seen in Fig. 9. (To increase readability, the yields for hydrogen and helium from ternary fissions are not shown.)

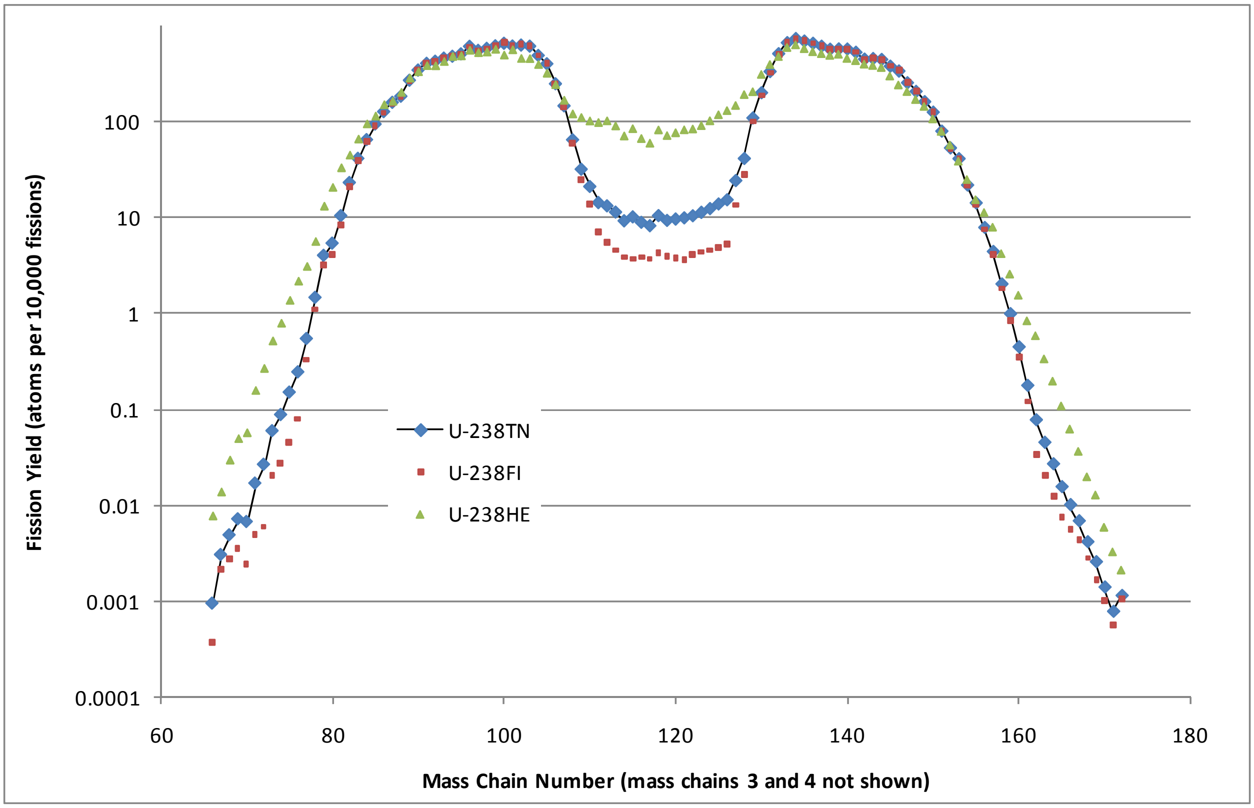


Fig. 9. Comparison of the new U238TN yield with the U238FI and U238HE yields.

2.2.4 Comparison with Crocker's Thermonuclear Yield

This weighting scheme is consistent with the logic used by Crocker to generate the original DELFIC U238TN yield, but it differs in practice. In 1963, Crocker used the yields of 21 nuclides as a guide to draw a smooth fission yield curve. This curve is notable in that it is symmetric and contains none of the minor perturbations evidenced in any of the other fission yield curves in the 1968 DELFIC data (Fig. 10).

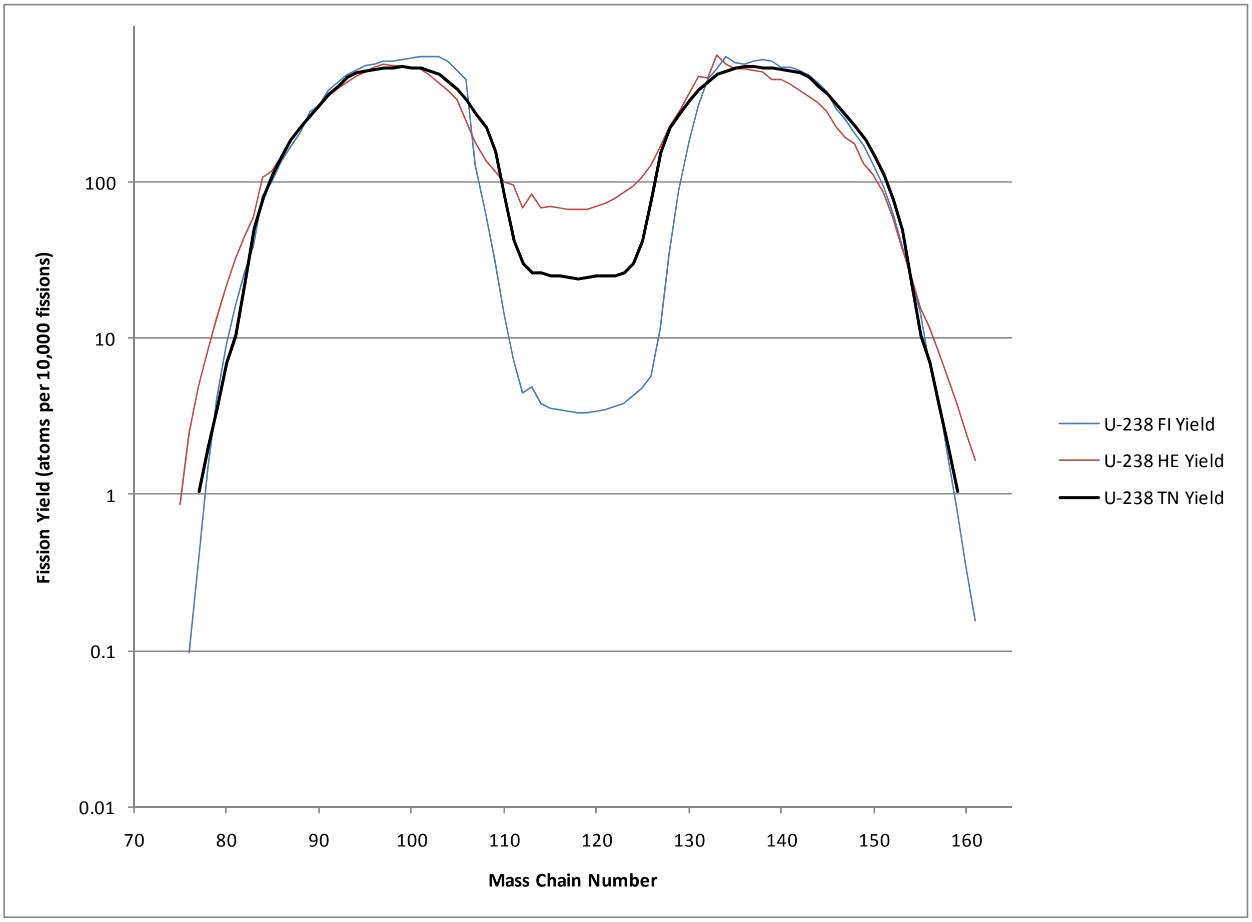


Fig. 10. Comparison of original ^{238}U yields in DELFIC.

After creating his thermonuclear yield curve, Crocker read the mass chain yield values and constructed individual nuclide yields based on the distribution in his 1963 report (Crocker 1963). The 1963 yields generated by Crocker differ slightly from the yields originally used in DELFIC. When compared side-by-side, the DELFIC yields tend to have very slightly larger mass chain yield values; for example, mass chain 99 had a yield of 545.6 in 1963, and a yield of 547.9 in DELFIC. Yet the shapes of the yields are effectively identical, as is seen in Fig. 11. (For clarity, the 1963 yield is illustrated as a dotted line so the reader may see both curves.)

The slight difference in values may be accounted for by the distribution of nuclides within the mass chains. For both yields, Crocker used a Gaussian distribution of nuclides about a theoretical most probable Z value (Zc) for each mass chain. The absolute deviation of a nuclide's Z value from the Zc for that chain determined the yield for that particular nuclide. When the 1963 and 1968 yields are compared within mass chains, the distribution of nuclides turns out to be identical, except for slightly different values of Zc. In Fig. 12 and Fig. 13, the distributions are compared for mass chains 99 and 137. In each chart, the distribution is identical relative to the Zc value of the mass chain. However, the Zc values are slightly different between 1963 and 1968. For example, in mass chain 99, the 1963 distribution is centered about a Zc value of 39.15 whereas the 1968 distribution is centered about a Zc value of 38.88. Likewise, the Zc values for the 137 mass chain are 52.85 in 1963 and 53.1 in 1968. The use of different Zc values causes the actual Z values to be located at different relative positions along the distribution, which then changes the values of the isotope yields. So while the distributions are identical shapes, the use of a different center affects individual isotopic yields within the mass chain.

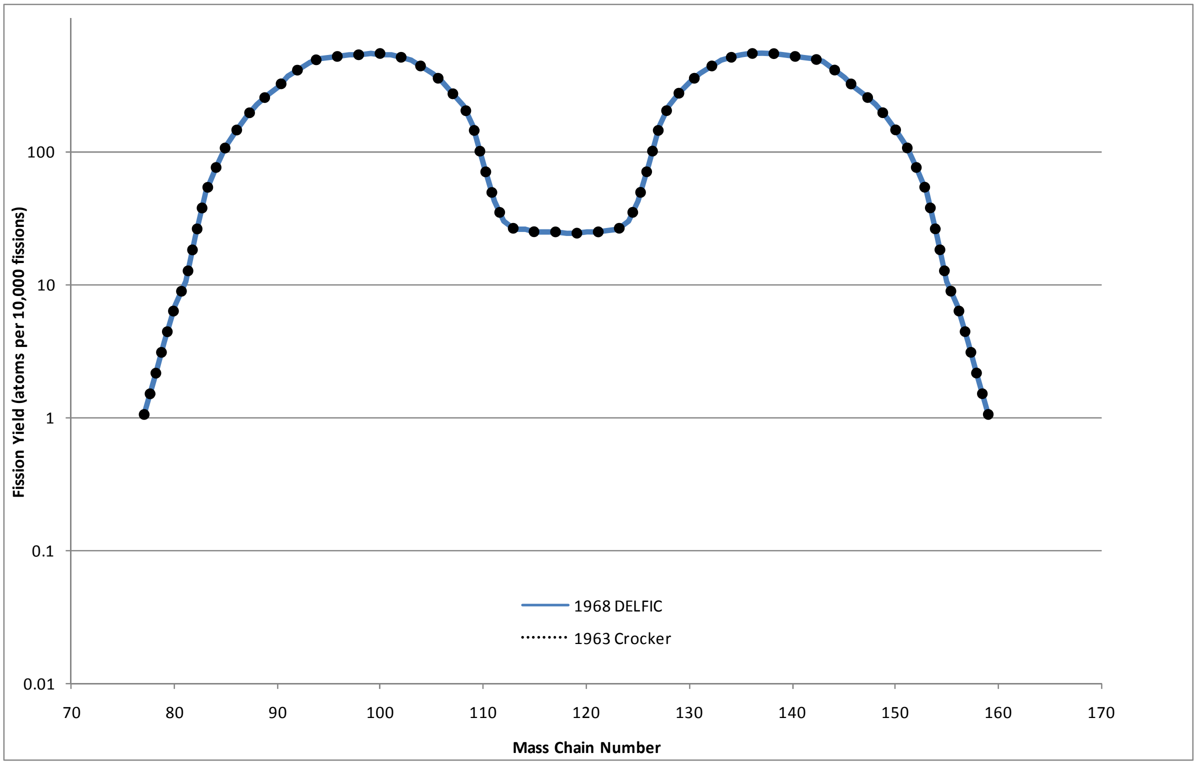


Fig. 11. Comparison of Crocker's U238TN yields in 1963 and 1968.

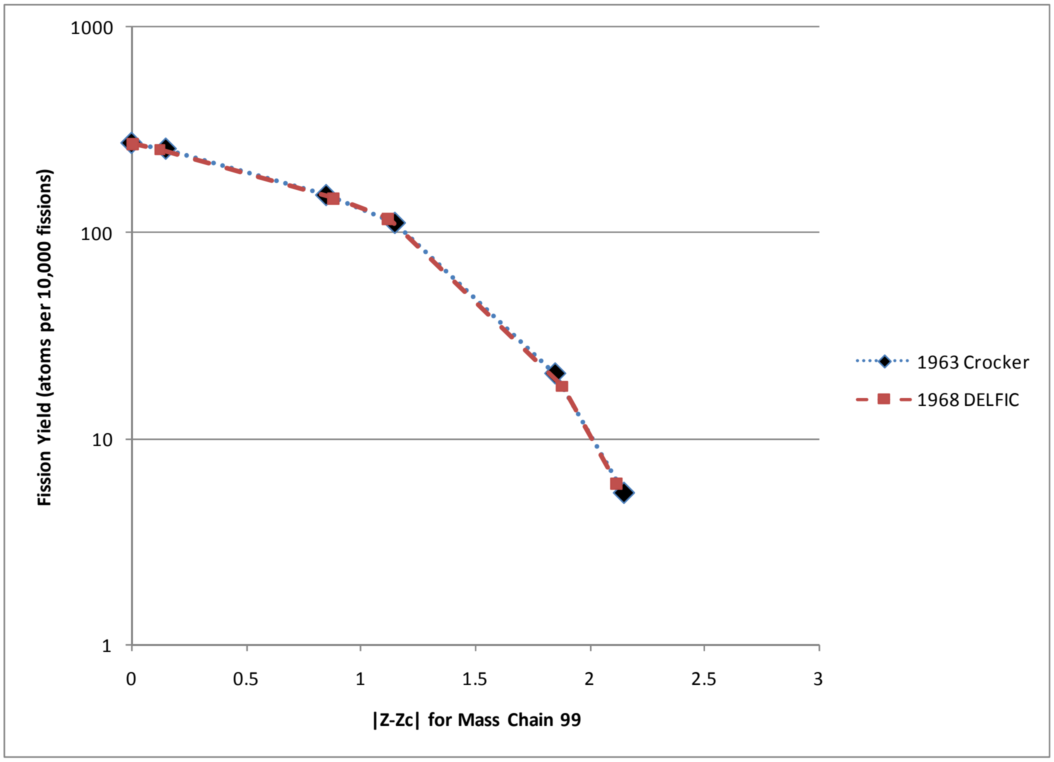


Fig. 12. Nuclide distribution within mass chain 99.

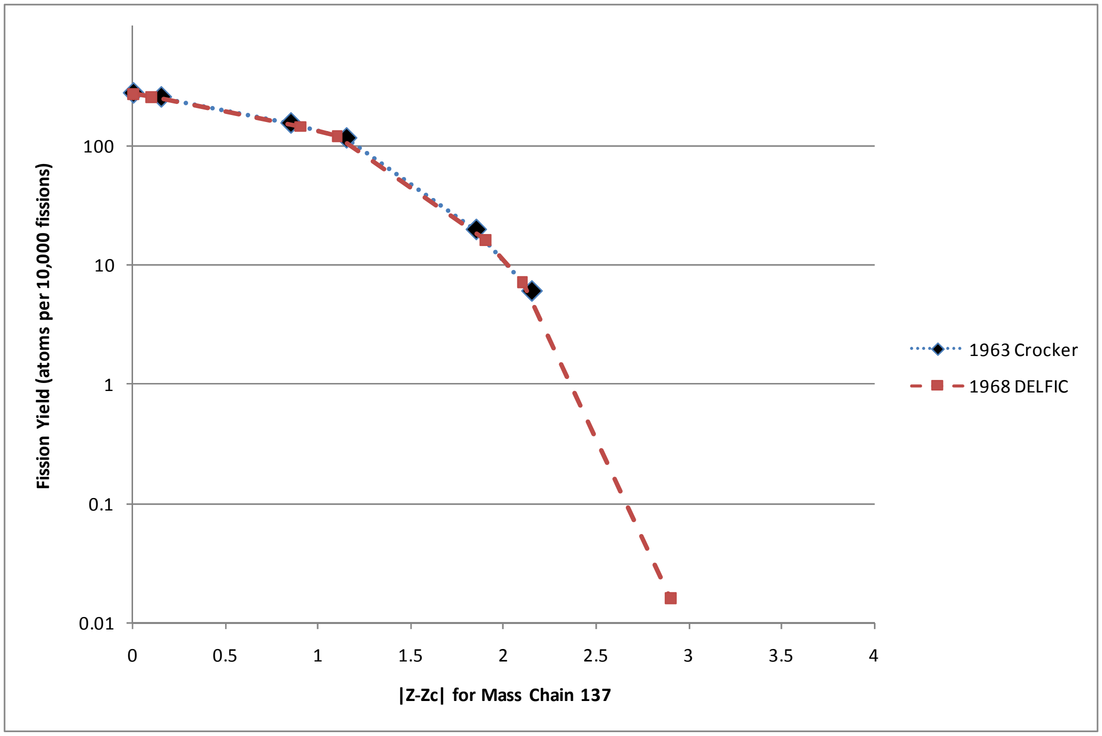


Fig. 13. Nuclide distribution within mass chain 137.

No information has yet been located to explain why Crocker used different Zc values in DELFIC. However, the total U238TN fission yield in 1963 adds to 19913.2 atoms per 10,000 fissions, whereas the yield in 1968 DELFIC adds to 19998.2 atoms per 10,000 fissions. The answer may simply be that Crocker wished to provide a yield that more accurately conserved fission products and adjusted the Zc values to optimize the yields.

In summary, the original U238TN yield in DELFIC was manufactured by plotting 21 measured nuclide yields, fitting a smooth, symmetric curve about those 21 points and filling in the gaps with interpolation between fission-energy and high-energy yields, then distributing the mass chain yields about a Gaussian distribution centered around a most probable Z value, Zc. The reason for the change in Zc values between 1963 and 1968 is not explicitly known but appears to be an attempt to better conserve fission products.

In 2008, there is a significant improvement in the fission yields for fission-energy and high-energy neutron spectra but not a significant improvement in the availability of thermonuclear yields. To generate the new thermonuclear yields, the values were interpolated between the fission-energy and high-energy spectra yields with the same weighting that Crocker originally used. However, the interpolation was performed on a nuclide-by-nuclide basis rather than a mass chain basis. This maximized the use of known yield information while keeping consistent with the theory that the thermonuclear yields may be accurately modeled through interpolation. Additionally, the new yields do not rely on hand-drawn curves.

Finally, as Crocker noted, the fission yields in a thermonuclear detonation will vary depending on the device properties, and some fission product yields may show very significant variation. With this in mind, the new 2008 thermonuclear yields—like the yields originally provided by Crocker—are an attempt to provide reasonable yields for DELFIC.

2.2.5 Branch Merging

Because of the past confusion over the matter of branch merging in DELFIC, treatment of branch merging in the new fission yields merits particular attention. In the past, branch merging was accounted for by three different methods: (1) in 1968, the subroutine YIELD accounted for branch merging every time the program was run; (2) in 1979, the fission yield data files were modified *a priori* to account for branch merging, and the subroutine YIELD was eliminated from the DELFIC code; and (3) in 1992, additional code lines were written to allocate the fission yields only once in the course of establishing the monolithic decay chains. All three methods are valid solutions to the problem of branch merging.

In this new version of DELFIC, the 1968 practice was followed. The YIELD subroutine was added back into DELFIC and adapted to handle the new yield and decay data. With this modification, the fission yields in TAPE2008.DAT are true fission yields, so they can be analyzed outside DELFIC without further modification.

2.2.6 Generation of BREAKUP.DAT

The new BREAKUP.DAT file was also created through the use of the ORIGEN-S card-image libraries and the data conversion program. With the ORIGEN data (Gauld, Murphy, and Williams 2006), the decay scheme was far more complex than in the original DELFIC decay scheme. The number of branches increased from 128 to 778. The number of b-n decays and electron capture/positron decays increased significantly. Alpha decays were available for the first time. The most intriguing addition was the occurrence of seemingly endless decay chains: beta decays to daughters that would, in turn, decay via electron capture back into the original parent. These differences necessitated revision of the coding in BREAKUP.DAT to handle the more complex chains and revisions of the ORIGEN decay data (performed by the data conversion program) to break the infinite loop of beta/electron capture decay cycles.

2.2.7 Decay Modes Update

The decay modes were significantly enhanced, both in the data tables and in the program logic. Most significantly, the methods used to read nuclidb in BATMAN were modified to allow 1 decay per nuclide with an increment greater than 7 but less than 64. Formerly, nuclidb used the bit convention in Fig. 14, which was identical to the rightmost five octal digits in the original NUCLID data. Since the daughter increments were restricted to 3 bits each, no decay increment greater than 7 could be represented. With the expanded list of nuclides and decay data in the ENDF/B-VII data, this precluded an unacceptably high number of decays and was probably the most significant reason that such an update had not been performed before.

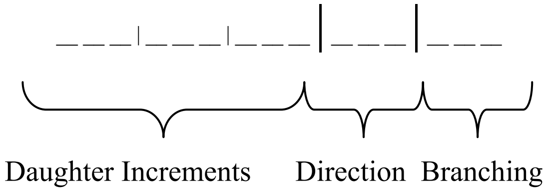


Fig. 14. Binary description of nuclidb.

The nuclidb word was modified as in Fig. 15.

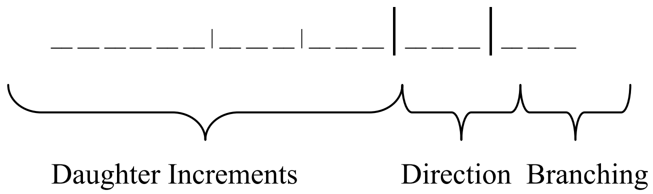


Fig. 15. Binary description of the modified nuclidb.

The first increment was expanded from a single octal digit to two octal digits (six total bits). The first decay branch could then increment up to 63 positions away from the parent nuclide, allowing for every b-n and every alpha decay in the ENDF/B-VII data and allowing for a full representation of the ENDF/B-VII decay modes.

Ideally, this modification would have been applied to all three daughter increments. Incorporating this change, however, would have required more extensive changes to the DELFIC logic and provided no immediate benefit; the current data do not contain any parent nuclides with multiple decays that increment by more than 7. For this reason, the simpler approach was adopted.

The branching ratio data were also updated with the new nuclide list. Formerly, DELFIC contained branching ratios for 128 branches; the new list accounts for 778 branches in the ENDF/B-VII data with space for up to 800. In both the old and new branching ratio data, the branching ratios were listed only for nuclides with multiple modes of decay (i.e., branching ratios of 1 were omitted). It should also be noted that the number of branches increases dramatically with more complex decay modes. If a future upgrade of the decay data should be performed, the maximum number of branching ratios might need to be increased accordingly.

The updates to the decay logic and nuclide inventory necessitated far more values in nuclidb than those in Table 2. A comprehensive list of the post-upgrade values in nuclidb is given in Table 10 (when the first increment is 8 or greater, the two octal digits are written in parentheses).

In the BATMAN and YIELD subroutines, DELFIC originally contained a decay chain length limit of 11 to end any accidental infinite decay loops. The number 11 was chosen according to the longest decay scheme in DELFIC at the time and served to close a hole that existed in the decay chain logic: nuclides with nuclidb (or originally, NUCLID) values of 0 caused a self-sustaining infinite DO-loop by appearing to the program logic as a nuclide that decays to itself. This occurred for every blank array position in the nuclide list, such as positions 693 through 700 in the original code. With the updated data, the maximum length of any decay chain is 10, so the length limit did not need to be revised from its original value.

2.3 BATEMAN EQUATION SINGULARITY

In the Bateman equations, a singularity develops whenever the decay constants of two nuclides in a decay chain have the same value. Because of the division of the difference of decay constants that occurs in various terms in the Bateman equations, a division by zero appears. To illustrate this problem, imagine a monolithic decay chain of 4 nuclides (3 unstable nuclides and 1 stable nuclide). The physical decay chain is represented in Fig. 16.

Table 10. nuclidb values after upgrade

nuclidb	nuclidb (octal digits)	Daughter increments	Number of occurrences	Common decay patterns
4	000|0|4	None	149	Stable
4100	100|0|4	+1	340	β^-
4132	100|4|4	–1	74	ε
4642	110|4|2	–1, +1	31	ε, IT
4769	112|4|1	–1, +1, +2	1	ε, IT, β^-
5122	120|0|2	+1, +2	78	IT, β^-
5154	120|4|2	–1, +2	1	ε, β^-
5634	130|0|2	+1, +3	13	IT, β^-
8196	200|0|4	+2	102	β^-
8228	200|4|4	–2	33	ε
8738	210|4|2	–2, +1	18	ε, β^-
8754	210|6|2	–2, –1	18	ε, ε
9730	230|0|2	+2, +3	3	β^-, β^-
12292	300|0|4	+3	7	β^-
13362	320|6|2	–3, –2	4	ε, ε
25122	610|4|2	–6, +1	5	β-n, β^-
29218	710|4|2	–7, +1	13	β-n, β^-
29730	720|4|2	–7, +2	2	β-n, β^-
30242	730|4|2	–7, +3	1	β-n, β^-
33314	(10)10|4|2	–8, +1	39	β-n, β^-
33441	(10)12|4|1	–8, +1, +2	2	β-n, IT, β^-
33505	(10)13|4|1	–8, +1, +3	1	β-n, IT, β^-
33826	(10)20|4|2	–8, +2	1	β-n, β^-
34338	(10)30|4|2	–8, +3	1	β-n, β^-
37410	(11)10|4|2	–9, +1	59	β-n, β^-
37537	(11)12|4|1	–9, +1, +2	1	β-n, IT, β^-
37922	(11)20|4|2	–9, +2	2	β-n, β^-
41506	(12)10|4|2	–10, +1	26	β-n, β^-
41633	(12)12|4|1	–10, +1, +2	1	β-n, IT, β^-
42018	(12)20|4|2	–10, +2	2	β-n, β^-
42530	(12)30|4|2	–10, +3	1	β-n, β^-
45602	(13)10|4|2	–11, +1	36	β-n, β^-
46114	(13)20|4|2	–11, +2	4	β-n, β^-
49698	(14)10|4|2	–12, +1	7	β-n, β^-
50210	(14)20|4|2	–12, +2	1	β-n, β^-
53794	(15)20|4|2	–13, +1	10	β-n, β^-
159780	(47)00|4|4	–39	1	α
160306	(47)10|6|2	–39, –1	2	α, ε
167972	(51)10|4|4	–41	1	α
172068	(52)10|4|4	–42	3	α
172594	(52)10|6|2	–42, –1	2	α, ε

$N_A \rightarrow N_B \rightarrow N_C \rightarrow N_D$

Fig. 16. Example decay chain.

In DELFIC, the decay chains are assembled locally for each monolithic chain; the solutions for each chain are then added back to the global solutions for each chain. To maintain this distinction, the alphabetical subscripts (A, B, C, and D) are used here to refer to the global nuclide terms, and numeric subscripts (1, 2, 3, and 4, respectively) are used to represent the local terms as compiled by DELFIC. The local decay chain would then appear as in Fig. 17.

$N_1 \rightarrow N_2 \rightarrow N_3 \rightarrow N_4$

Fig. 17. Example localized decay chain.

The local construction of the Bateman equation for nuclide 3 (global nuclide C) produces the result in Equation 2.

$$N_3(t) = \frac{\lambda_2\lambda_1}{\boldsymbol{(\lambda_3 - \lambda_1)}(\lambda_2 - \lambda_1)} N_{1,0} e^{-\lambda_1 t} + \frac{\lambda_2}{\lambda_3 - \lambda_2} N_{2,0} e^{-\lambda_2 t} + \frac{\lambda_2\lambda_1}{(\lambda_3 - \lambda_2)(\lambda_1 - \lambda_2)} N_{1,0} e^{-\lambda_2 t}$$
$$+ N_{3,0} e^{-\lambda_3 t} + \frac{\lambda_2}{\lambda_2 - \lambda_3} N_{2,0} e^{-\lambda_3 t} + \frac{\lambda_2\lambda_1}{(\lambda_2 - \lambda_3)\boldsymbol{(\lambda_1 - \lambda_3)}} N_{1,0} e^{-\lambda_3 t}$$

Equation 2. Bateman equation for nuclide C.

Suppose that the decay constants for nuclides 1 and 3 are equal, while the decay constant for nuclide 2 is significantly different. ("Significantly different," for the sake of the original DELFIC code, means that the decay constant of nuclide 2 is different from those of 1 and 3 by at least 10^{-15} s^{-1}. The explanation for this will follow shortly.) Two terms would then contain a division by 0 (shown in Equation 2 in red). Mathematically, these two terms cancel exactly and the singularity disappears. However, the sequential construction of the equation cannot perfectly account for the limit, and the solution would be invalid. To circumvent the singularity, DELFIC includes the two lines of code shown in Fig. 18.

```
FACTC=SDC(K2)-SDC(K1)
IF(ABS(FACTC).LT.1.E.-15) FACTC=SIGN(1.E.-15,FACTC)
```

Fig. 18. DELFIC code to circumvent the singularity.

The first line in Fig. 18 establishes the differences of decay constants (for example, as seen in red in Equation 2). If the magnitude of difference is less than 10^{-15}, the second line of code replaces the difference with the value 10^{-15} and applies the sign of the difference. Theoretically, this adjustment creates zero error. The cancellation can be seen in Equation 3, where the remaining terms are overlooked for simplicity.

$$N_3(t) = \frac{\lambda_2\lambda_1}{\boldsymbol{(\lambda_3 - \lambda_1)}(\lambda_2 - \lambda_1)} N_{1,0} e^{-\boldsymbol{\lambda_3} t} + \frac{\lambda_2\lambda_1}{(\lambda_2 - \lambda_3)\boldsymbol{(\lambda_1 - \lambda_3)}} N_{1,0} e^{-\lambda_3 t} + \cdots$$

Equation 3. Bateman equation, focusing on the singularity terms.

Note that in Equation 3, λ_1 has been replaced with λ_3 in the exponent of the first term (in blue). Mathematically, these terms cancel, as the limit of ($\lambda_3 - \lambda_1$) approaches 0. However, the SIGN function used in the second line of code in Fig. 18 always applies a positive sign when the term FACTC is exactly 0. With this substitution, Equation 3 appears as in Equation 4.

$$N_3(t) = \frac{\lambda_2\lambda_1}{\mathbf{10^{-15}}(\lambda_2 - \lambda_1)} N_{1,0} e^{-\lambda_3 t} + \frac{\lambda_2\lambda_1}{(\lambda_2 - \lambda_3)\mathbf{10^{-15}}} N_{1,0} e^{-\lambda_3 t} + \cdots$$

Equation 4. Bateman equation with the perturbation of the singularity.

Rather than cancelling the two terms, DELFIC *adds* the terms. The logical flaw has existed in DELFIC since 1968. Despite at least 25 occurrences of the singularity in the original DELFIC nuclide data, the error never appeared significant for a gratuitous reason. In all cases of the singularity, the two decay constants equaled 69.31472 s^{-1} (equivalent to a half life of 0.01 s). When the values for the decay constants were substituted into the equations, the exponential factors drove the two singularity terms to insignificance, as seen in Equation 5.

$$N_3(t) = \frac{\lambda_2\lambda_1}{\mathbf{10^{-15}}(\lambda_2 - \lambda_1)} N_{1,0} e^{-\mathbf{69.31472}t} + \frac{\lambda_2\lambda_1}{(\lambda_2 - \lambda_3)\mathbf{10^{-15}}} N_{1,0} e^{-\mathbf{69.31472}t} + \cdots$$

Equation 5. Bateman equations with substituted decay constant values.

In the 2008 data, the decay constants for ^{122m}Ag and ^{122}In are both equal to 4.62098E–01 s^{-1} and create the mathematical singularity. Unlike the occurrences of the singularity in the 1968 data, the exponential factors do not drive the singularity terms to insignificance. Instead, these terms dominate the Bateman equation, as seen in Equation 6 (for readability, the global subscripts are used).

$$N_3(t) = \frac{\lambda_2\lambda_1}{\mathbf{10^{-15}}(\lambda_2 - \lambda_1)} N_{1,0} e^{-\mathbf{0.462098}t} + \frac{\lambda_2\lambda_1}{(\lambda_2 - \lambda_3)\mathbf{10^{-15}}} N_{1,0} e^{-\mathbf{0.462098}t} + \cdots$$

Equation 6. Bateman equations focusing on the singularity for ^{122m}Ag and ^{122}In.

The 10^{-15} factors in the denominators caused the two perturbed terms to have values several orders of magnitude greater than the other terms in the equation (in some observed cases, as many as 12 orders of magnitude greater). Even if the signs were correctly applied, the values of the other terms of the equations would be lost because of a lack of precision.

To correct the problem with the singularity, two changes were made to the code in Fig. 18. First, for cases where the term FACTC (the difference between two decay constants found in the denominator for a term) equaled exactly 0, the term was multiplied by –1, but only if K2 was less than K1. The negative sign would then be applied only to the second term in Equation 6. Second, the substitution value was increased from 10^{-15} to 1. Increasing the substitution value reduced the value of the entire term, eliminating the precision error in the equation.

As a third adjustment, the threshold value for the substitution of FACTC was reduced from 10^{-15} to 10^{-30}. The reduction was made because of a valid difference in decay constants between ^{113}Cd and ^{113}In of 2.85352E–24 s^{-1}. Though both nuclides are effectively stable for the time frame of concern in fallout modeling, lowering the threshold for substitution removed the unnecessary introduction of a perturbation when the decay constants were not exactly equal (and the two terms did not exactly cancel). To help improve the overall precision of the Bateman equations (particularly for these nuclides), all terms in the Bateman equations were converted to double precision.

2.4 CONSERVATION OF FISSION PRODUCTS

After the preceding changes were introduced, DELFIC was tested for conservation of nuclides. The total nuclide abundances for three yields with fission neutron spectra are shown in Table 11. The times evaluated were the soil solidification times for siliceous soil for a 1 kt yield (2.3161 s), a 1-Mt yield (9.4598 s) and 1 h.

Table 11. Total nuclide abundances for various fission types

	Fission type	TAPE2008.DAT	t = 2.3161 s	t = 9.4598 s	t = 3600 s
Abundance (atoms per 10,000 fissions)	U238FI	20018.83	20019.70	20019.71	20019.70
	U235FI	20023.84	20024.64	20024.59	20024.63
	Pu239FI	20026.79	20027.42	20027.42	20027.37

The abundances sum to slightly higher than 20,000 fission products per 10,000 fissions as a result of the contribution of ternary fissions. (For example, the fission yield of U238FI includes 18.33 hydrogen and helium fission products. If the fissions that produced those products had been binary rather than ternary fissions, then the fission yield would have been 20000.50—less than one atom error for 10,000 fissions.) Overall, the deviation from pure conservation was less than 1 atom per 10,000 fissions regardless of the time at which the abundances were recorded.

2.4.1 Input Deck Control

The abundances of the fission products can be printed by use of a control integer in the output processor module (OPM) input deck. In the OPM deck, card 2 consists of twenty 4 digit integers assigned to the array IC(20). Previously, DELFIC used only the first two array positions in IC. In the 2008 upgrade, the third array position was assigned as the control switch for printing the nuclide abundances. If IC(3) is greater than 0 *and* if NPRNT(9) is set to true, a list of the nuclides and their abundances (in units of atoms per 10,000 fissions) will follow the list of nuclide activities.

2.5 EXPOSURE RATE MULTIPLIERS

To approximate the exposure rates due to fallout, DELFIC uses conversion factors termed ERMs. The activity rates of the fission products and their daughters are multiplied by ERMs, converting the output from disintegrations/s to R/h. ERMs are similar in concept to *dose conversion factors* in that they estimate the exposure rate at a given point for a given geometry. For ERMs, exposure for a given nuclide is estimated at 1 m above a perfectly smooth and flat infinite plane with a uniform distribution of the nuclide on the surface of the plane. (DELFIC, by the user-supplied value for GRUFF, accounts for surface roughness by reducing the exposure rates of all nuclides.)

In 1979, DELFIC contained ERMs for only 181 of the 692 nuclides in its inventory (108 of the 692 are stable). Although many other radioactive nuclides were gamma emitters and therefore contributed to exposure rates, their contributions to exposure rates were neglected—most likely because of a lack of information for those nuclides. In 1992, SAIC generated a new set of ERMs as a part of its work on DELFIC. The 1992 ERMs contained nonzero values for 574 of the 692 nuclides, as well as 171 nuclides not included in the list of 692 nuclides. In brief, the SAIC ERMs were based on ENDF/B-VI and solved through the use of the ANISN transport code. In 2008, work was performed by Eckerman of ORNL to calculate a new list of ERMs (Eckerman 2008). Eckerman's work provided ERMs for many of the original 692 nuclides in DELFIC, as well as many of the additional nuclides in the 2008 inventory of 1096 nuclides and many nuclides not included in either inventory. Like their predecessors, Eckerman's ERM values were calculated at a point 1 m above an infinite plane with no ground roughness, assuming a uniform distribution of the nuclide for each ERM.

2.5.1 Comparison of ERMs

The ERMs were compared by looking solely at the ERMs associated with the 692 nuclides found in the 1979 and 1992 data sets. The 2008 inventory contains many ERM values for nuclides not found in the 692 nuclides; these additional ERMs will be ignored here for the sake of comparing values for common nuclides. A brief summary is given in Table 12.

Table 12. General differences among ERM data

	ERMs for 1979 DELFIC nuclides		
	1979	**1992**	**2008**
Number of ERMs	181	574	574
Maximum	1.80E–05	1.95E–05	2.30E–05
Minimum	1.73E–08	0.00E+00	0.00E+00
Mean	3.40E–06	6.06E–06	6.50E–06
Median	2.03E–06	5.56E–06	5.85E–06

The 2008 ERMs included a value for most radioactive nuclides, as did the 1992 version. The 1979 ERMs tended to focus on the last two or three radioactive nuclides in each mass chain; these nuclides are the most important for exposure calculations, as the other radioactive nuclides will eventually decay into them (Table 13).

Table 13 shows that when the ERMs were upgraded from 1979 to 1992 by SAIC, the most significant differences tended to raise the value of the ERMs, resulting in a higher exposure rate approximation. In fact, of the top 20 differences in ERM values (by percentage difference relative to the 1979 values), all of the 1992 ERMs were greater than their 1979 counterparts. However, the values of the twenty 1979 ERMs all fell below the 1979 average of 3.40E–06, and 17 of the twenty 1992 ERMs fell below the 1992 average of 6.06E–06. This suggests that the major changes in ERMs in 1992 did not greatly affect the larger ERM values. The most significant changes (in absolute terms) were to ^{93}Sr and ^{140}Cs.

Similar to the 1992 ERMs, the 2008 ERMs were greater in value than their 1979 equivalents (by percentage difference) for 19 of the top 20 ERM changes (seen in Table 14). Overall, the ERM values for the 2008 data tended to fall between the 1979 and the 1992 values.

In 1992 and 2008, 15 of the top 20 changes in the ERM values with respect to the 1979 values were common for ^{97}Zr, ^{93}Sr, ^{83m}Se, ^{125}Sn, ^{79m}Se, ^{81m}Se, ^{104m}Rh, ^{131}Sb, ^{109m}Ag, ^{139}Xe, ^{160}Tb, ^{140}Cs, ^{105}Rh, ^{153}Sm, and ^{125m}Te (Table 15). In all 15 cases, the ERMs increased from their 1979 values.

Table 13. Differences in ERMs from 1979 to 1992

Nuclide	$t_{1/2}$ (hr)	$\beta_{cumulative}$ (atoms per 10^4 fissions)	Top 20 differences in ERM values for common nuclides: 1979 and 1992			
			ERM values		1979–1992	
			1979	1992	Difference	(%)
^{93}Sr	1.24E–01	5.00E+00	1.14E–06	1.04E–05	–9.22E–06	808%
^{83m}Se	1.95E–02	2.78E–01	6.66E–07	4.29E–06	–3.63E–06	545%
^{111m}Pd	5.50E+00	1.47E–06	3.40E–07	1.89E–06	–1.55E–06	456%
^{97}Zr	1.69E+01	5.57E+00	2.38E–07	9.08E–07	–6.70E–07	282%
^{125}Sn	2.31E+02	5.97E–03	3.98E–07	1.41E–06	–1.01E–06	254%
^{79m}Se	6.53E–02	3.32E–02	1.04E–07	3.13E–07	–2.09E–07	201%
^{160}Tb	1.74E+03	1.16E–05	2.02E–06	5.89E–06	–3.87E–06	192%
^{140}Cs	1.77E–02	5.96E+00	3.23E–06	9.01E–06	–5.78E–06	179%
^{139}Xe	1.10E–02	5.55E+00	1.46E–06	4.06E–06	–2.60E–06	178%
^{81m}Se	9.55E–01	2.19E–03	1.15E–07	3.20E–07	–2.05E–07	178%
^{119m}In	3.00E–01	2.59E–04	2.69E–07	7.39E–07	–4.70E–07	175%
^{109m}Ag	1.10E–02	2.68E–03	8.05E–08	2.09E–07	–1.28E–07	160%
^{131}Sb	3.84E–01	3.19E+00	3.18E–06	8.01E–06	–4.83E–06	152%
^{153}Sm	4.63E+01	4.11E–01	1.86E–07	4.68E–07	–2.82E–07	152%
^{104m}Rh	7.23E–02	7.43E–10	2.15E–07	5.30E–07	–3.15E–07	146%
^{107}Ru	6.25E–02	1.30E+00	1.22E–06	2.95E–06	–1.73E–06	142%
^{105}Rh	3.54E+01	3.94E+00	1.75E–07	4.17E–07	–2.42E–07	138%
^{125m}Te	1.38E+03	1.15E–04	3.27E–07	7.55E–07	–4.28E–07	131%
^{108}Rh	4.67E–03	5.98E–01	2.36E–06	5.36E–06	–3.00E–06	127%
^{112}Pd	2.10E+01	6.50E–04	1.25E–07	2.81E–07	–1.56E–07	125%

Table 14. Differences in ERMs from 1979 to 2008

Nuclide	$t_{1/2}$ (hr)	$\beta_{cumulative}$ (atoms per 10^4 fissions)	Top 20 differences in ERM values for common nuclides: 1979 and 2008			
			ERM values		1979–2008	
			1979	2008	Difference	(%)
^{97}Zr	1.69E+01	5.57E+00	2.38E–07	4.49E–06	–4.25E–06	1787%
^{93}Sr	1.24E–01	5.00E+00	1.14E–06	1.11E–05	–9.94E–06	872%
^{83m}Se	1.95E–02	2.78E–01	6.66E–07	4.74E–06	–4.07E–06	612%
^{125}Sn	2.31E+02	5.97E–03	3.98E–07	1.63E–06	–1.23E–06	310%
^{79m}Se	6.53E–02	3.32E–02	1.04E–07	3.80E–07	–2.76E–07	266%
^{81m}Se	9.55E–01	2.19E–03	1.15E–07	4.01E–07	–2.86E–07	249%
^{104m}Rh	7.23E–02	7.43E–10	2.15E–07	6.88E–07	–4.73E–07	220%
^{131}Sb	3.84E–01	3.19E+00	3.18E–06	1.00E–05	–6.82E–06	214%
^{109m}Ag	1.33E–02	2.68E–03	8.05E–08	2.51E–07	–1.70E–07	211%
^{139}Xe	1.10E–02	5.55E+00	1.46E–06	4.24E–06	–2.78E–06	190%

Table 14. (continued)

Nuclide	$t_{1/2}$ (hr)	$\beta_{\mathrm{cumulative}}$ (atoms per 10^4 fissions)	Top 20 differences in ERM values for common nuclides: 1979 and 2008			
			ERM values		1979–2008	
			1979	2008	Difference	(%)
^{160}Tb	1.74E+03	1.16E–05	2.02E–06	5.61E–06	–3.59E–06	178%
^{140}Cs	1.77E–02	5.96E+00	3.23E–06	8.02E–06	–4.79E–06	148%
^{119m}Sn	7.03E+03	1.11E–06	1.47E–07	3.56E–07	–2.09E–07	143%
^{105}Rh	3.54E+01	3.94E+00	1.75E–07	4.01E–07	–2.26E–07	129%
^{102m}Tc	7.25E–02	1.28E–04	5.35E–06	1.18E–05	–6.42E–06	120%
^{149}Pm	5.31E+01	1.61E+00	2.80E–08	6.15E–08	–3.35E–08	120%
^{153}Sm	4.63E+01	4.11E–01	1.86E–07	4.05E–07	–2.19E–07	118%
^{116m}Ag	2.39E–03	7.72E–04	6.43E–06	1.32E–05	–6.78E–06	105%
^{125m}Te	1.38E+03	1.15E–04	3.27E–07	6.70E–07	–3.43E–07	105%
^{104}Rh	1.18E–02	9.55E–10	3.00E–06	6.66E–08	2.93E–06	98%

Table 15. Differences in ERMs from 1992 to 2008

Nuclide	$t_{1/2}$ (hr)	$\beta_{\mathrm{cumulative}}$ (atoms per 10^4 fissions)	Top 20 differences in ERM values for common nuclides: 1992 and 2008			
			ERM values		1992–2008	
			1992	2008	Difference	(%)
^{109}Pd	1.37E+01	2.68E–01	3.36E–09	2.55E–07	–2.52E–07	7484%
^{97}Zr	1.69E+01	5.57E+00	9.08E–07	4.49E–06	–3.58E–06	395%
^{102}Tc	1.47E–03	6.32E+00	4.73E–06	4.04E–07	4.33E–06	91%
^{152}Pm	1.14E–03	4.82E–01	7.38E–07	1.41E–06	–6.73E–07	91%
^{111m}Pd	5.50E+00	1.47E–04	1.89E–06	2.42E–07	1.65E–06	87%
^{114}Pd	4.03E–02	3.93E–02	4.48E–07	1.34E–07	3.14E–07	70%
^{108}Rh	4.67E–03	5.98E–01	5.36E–06	1.66E–06	3.70E–06	69%
^{102}Mo	1.88E–01	6.32E+00	2.56E–07	9.46E–08	1.61E–07	63%
^{115m}Cd	1.07E+03	2.69E–03	5.64E–06	2.27E–06	3.37E–06	60%
^{99m}Nb	4.33E–02	2.22E+00	7.11E–06	3.42E–06	3.69E–06	52%
^{126}Sn	8.77E+08	6.30E–02	8.99E–07	4.41E–07	4.58E–07	51%
^{153}Pm	1.46E–03	4.11E–01	8.93E–07	4.40E–07	4.54E–07	51%
^{119m}In	3.00E–01	2.59E–02	7.39E–07	3.65E–07	3.74E–07	51%
^{99}Mo	6.59E+01	6.20E+00	1.42E–06	7.86E–07	6.35E–07	45%
^{103m}Rh	9.35E–01	6.19E–02	3.91E–08	5.58E–08	–1.67E–08	43%
^{113m}Ag	1.91E–02	6.44E–06	6.39E–07	3.69E–07	2.71E–07	42%
^{107}Ru	6.25E–02	1.30E+00	2.95E–06	1.73E–06	1.22E–06	41%
^{147}Pr	2.23E–01	2.53E+00	4.37E–06	2.65E–06	1.72E–06	39%
^{151}Sm	7.89E+05	8.06E–01	1.64E–10	2.28E–10	–6.35E–11	39%
^{114}Ag	1.28E–03	3.94E–02	9.21E–07	1.26E–06	–3.38E–07	37%

Comparing the 2008 and 1992 ERMs, the differences between ERM values tend to be slightly smaller than those between the 2008 and 1979 data. The two most significant changes were to ^{109}Pd and ^{97}Zr, where the 2008 ERMs were substantially greater than in 1992. The change to ^{97}Zr is particularly noteworthy; it is a nuclide with a relatively large fission yield and a half-life on the order of an hour, so the increase in the ERM value may influence exposure rates shortly after a detonation.

2.5.2 Exposure Rate Comparison between 1979 and 2008 ERMs

The effect of changing the ERM values was compared with the 1979 version of DELFIC using the test case input deck provided in the 1979 documentation. In this case, a 50-kt shot was detonated with a 100% fission yield and a ^{239}Pu high-energy neutron fission spectrum. Map option 2 was requested, which provided the exposure rate at 1 h after the detonation assuming that all fallout had reached the ground. All input conditions and requests were identical. In 1979, the sum of the exposure rates of the map ordinates was 0.285505E+05 R/h; in 2008, the sum of the exposure rates of the map ordinates was 0.279520E+05, a reduction of 2.40%. The peak value at an individual map ordinate occurred at the same location for both cases: 1.302E+03 R/h for the 1979 version and 1.235E+03 R/h for the 2008 version—a reduction of 5.15%. The proportional differences tended to be small among the map ordinates with larger values (i.e., the map ordinates along the centerline of the fallout pattern).

2.5.3 Summary Details of 2008 ERMs

Of the 1096 nuclides in the 2008 DELFIC fission yield database, 149 are stable nuclides. An additional 34 nuclides have ERM values of 0.00; most of these (e.g., ^{90}Sr) have no associated gamma and therefore no direct contribution to exposure. The remaining 913 nuclides have nonzero ERM values and are potential contributors to exposure. Many of these nuclides, however, exist at the beginning of their mass chains (e.g., ^{109}Zr); their very short half-lives and small cumulative yields prevent them from being significant contributors to exposure after a short period (e.g., 1 h).

3. PROPOSED AND PENDING WORK

3.1 INTRODUCTION

Several areas of the DELFIC Particle Activity Module can reasonably be updated from prior versions—particularly the stored data. The following section discusses a few topics (with justifications) for upgrade. These are topics that have not been upgraded as of the printing of this report but are recommended for future work to improve the accuracy and functionality of DELFIC.

3.2 DOSIMETRY

One of the primary functions of DELFIC is to model the exposure rates from ground-based fallout as a function of time and location relative to ground zero. The OPM was originally written to provide data and maps for instantaneous exposure rates and integrated exposure in units of Roentgens per hour and Roentgens, respectively. Owing to a lack of complete data, DELFIC was originally written to calculate exposure rates from only 181 nuclides. In 1992, SAIC improved the original exposure calculations by including ERM data for all radioactive nuclides within the original set of 692 fission products. However, upgrading the fission yield database has introduced many additional radioactive nuclides that contribute to exposure. The work performed by Eckerman (2008) has provided ERM values consistent with the ENDF/B-VII decay data as found in ORIGEN.

Creation of a dose conversion factor database is also proposed. Since contemporary radiological practices tend to favor effective dose rate measurements (e.g., rem/h) over exposure rate measurements (e.g., R/h), a second multiplier database should be created to allow the direct calculation of predicted effective dose rates. Since it is assumed that effective dose calculations could be conducted by the same logic that currently calculates exposure rates, little modification would be required of the current DELFIC code to provide effective dose calculation outputs.

3.3 INDUCED ACTIVITY

For all explosions other than pure airbursts, DELFIC calculates the activity induced in the lofted soil based on the soil composition, the amount of soil included in the radioactive cloud, and the yield of the explosion. Activity inducement is not calculated directly; DELFIC models the interaction of fission neutrons with the soil through a database of empirical values based on past observation. The method used by DELFIC is very computationally efficient and requires very little memory, as was common for computer codes in the 1960s. The code could easily be upgraded, however, to include more detail about soil composition and soil/radiation interaction.

Owing to time constraints, upgrading the induced activity calculations was not investigated during the research described in this paper. However, revisions to the fission product data and decay model have proved to be beneficial to DELFIC; revising the induced activity calculations would be a very reasonable step to improving the modeling capability of DELFIC.

3.4 ACTINIDES

After the fission event, actinide nuclides exist as a result of incomplete fuel burnup and transmutation of fuel atoms. These nuclides begin decay chains known to release a significant amount of gamma, beta, neutron, and alpha radiation. The contribution of actinides to the overall fallout radiation is currently modeled in a subroutine called URAN. URAN considers only the decay of ^{239}U and ^{239}Np in its calculations, although several other isotopes (including isotopes of U, Np, Pu, Am, and Cm) are known to exist after a fission event.

The modeling of the production and decay of actinides could be significantly enhanced by expanding the database of actinides and by improving the decay and radiation modeling within the subroutine URAN. Since computer processing time and memory are not as restrictive as they were during the 1960s, this is an upgrade to DELFIC that could significantly improve its fallout model without causing an undue burden on computer resources.

3.5 FRACTIONATION

DELFIC currently models fractionation in the subroutine FRATIO by determining which nuclides (or rather, oxides of nuclides) will have condensed by the time of soil solidification for a particular fission event. If the nuclides have sufficiently high boiling points to condense before soil solidification occurs, they are included throughout the volumes of the particles rather than along the surfaces.

The boiling point data for the oxides of the nuclides have been upgraded to include boiling points for all elements/oxides from hydrogen to curium. By storing boiling points for elements other than the fission products, fractionation may be expanded to include actinides and induced elements. If the inputs were to include data on the soil composition and the presence of actinides, FRATIO could easily be upgraded to incorporate their contribution to the radioactivity of the fallout particles.

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